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FILE COVERS 1907 - 15 Oct 2008 VOL 149 ISS 16 FILE LAST UPDATED: 14 Oct 2008 (20081014/ED)

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Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

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=> s 15
L8
            20 L5
=> s 18 not (2008/so or 2007/so or 2006/so or 2005/so)
        657090 2008/SO
       967291 2007/SO
       945741 2006/SO
        884922 2005/SO
            19 L8 NOT (2008/SO OR 2007/SO OR 2006/SO OR 2005/SO)
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     (FILE 'HOME' ENTERED AT 10:15:37 ON 15 OCT 2008)
     FILE 'REGISTRY' ENTERED AT 10:15:43 ON 15 OCT 2008
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             50 S L1
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          75421 S 5-6-7/SZ
L5
            446 S L3 AND L4
L6
            302 S L5 AND CAPLUS/LC
L7
            144 S L5 NOT L6
     FILE 'CAPLUS' ENTERED AT 10:18:18 ON 15 OCT 2008
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             19 S L8 NOT (2008/SO OR 2007/SO OR 2006/SO OR 2005/SO)
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L1 HAS NO ANSWERS
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L9 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:174325 CAPLUS

DOCUMENT NUMBER: 146:251874

TITLE: Preparation of tricyclic β -secretase inhibitors

for the treatment of Alzheimer's disease

INVENTOR(S): Nantermet, Philippe G.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 32pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: Facent English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

						D	DATE			APPL	ICAT	DATE					
	2007				A2 20070215				WO 2	006-							
WO		07019078					20070712										
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE.	GH.	GM.	HN.	HR.	HU,	ID,	IL.	IN.	IS.	JP.	KE.	KG.	KM.	KN.	KP.
								LS,									
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							ZM.		,	,	,	,	,	,	,	,	,
	RW:	AT.	BE.	BG.	CH.	CY.	CZ.	DE,	DK.	EE.	ES.	FI.	FR.	GB.	GR.	HU.	IE.
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PRIORITY APPLN. INFO.:										US 2	005-	/052.	28P		P 2	0050	803
OTHER SOURCE(S): GI						PAT	146:	2518	74								

AB Title compds. [I; X = oxadiazolylene, oxazolylene, imidazolylene, thiazolylene, isoxazolylene, aminopyrimidinylene, furylene; A = H, (substituted) alkyl, alkenyl; Q = (substituted) alkylene; R1 = (substituted) aryl, heteroaryl, alkyl; R2 = OH, amino; R3, R4 = alkyl, alkenyl, halo, alkoxy, amino, cyano, OH; m, n = 0-2; p = 1, 2; Y1Y2 = NR5SO2, NR5CO; R5 = H, alkyl, alkenyl, alkynyl, cyloalkyl, aryl, heteroaryl, aralkyl, heteroarylakyl, arylcycloalkyl, aryl, heteroarylcycloalkyl; Y3Y4Y5 = NCR8:CR9; R8 = H, alkyl, cycloalkyl; R9 = H, alkyl, cycloalkyl, aryl, heteroarylakyl, aryl, heteroarylakyl, tetc.], were prepared Thus, (2R)-2-[5-(7-ethyl-1-methyl-2,2-dioxido-3,4-dihydro-1H-

1,2,5-thiadiazepino[3,4,5-hi]indol-9-y1)-1,3,4-oxadiazol-2-y1]-1-phenylpropan-2-amine [preparation from Me

7-ethyl-1-methyl-3,4-dihydro-1H-1,2,5-thiadiazepino[3,4,5-hi]indole-9-carboxylate 2,2-dioxide, a-methyl-D-phenylalanine, and tert-Bu carboxate qiven] inhibited B-secretase with an IC50 of between 1 nM

and 100 μM. 925455-50-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of tricyclic β -secretase inhibitors for the treatment of Alzheimer's disease)

RN 925455-50-1 CAPLUS

CN 1,3,4-0xadiazole-2-methanamine, 5-(7-ethyl-3,4-dihydro-1-methyl-2,2-dioxido-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepin-9-yl)-α-methyl-α-(phenylmethyl)-, (αR) - (CA INDEX NAME)

Absolute stereochemistry.

IT 790254-40-9P 790254-64-7P 925455-51-2P

925455-52-3P 925455-53-4P 925455-54-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tricyclic β -secretase inhibitors for the treatment of Alzheimer's disease)

RN 790254-40-9 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-methyl-, methyl ester, 2,2-dioxide (CA INDEX NAME)

- RN 790254-64-7 CAPLUS
- CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

- RN 925455-51-2 CAPLUS
- CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dlhydro-1-methyl-, 2-[(1,1-dimethylethoxy)carbonyl]hydrazide, 2,2-dioxide (CA INDEX NAME)

- RN 925455-52-3 CAPLUS
- CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-methyl-, hydrazide, 2,2-dioxide (CA INDEX NAME)

RN 925455-53-4 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-methyl-, 2-[2-[[1,1-dimethylethoxy)carbonyl]amino]-2-methyl-1-oxo-3-phenylpropyl]hydrazide, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

- RN 925455-54-5 CAPLUS
- CN Carbamic acid, N-[(1R)-1-[5-(7-ethyl-3, 4-dihydro-1-methyl-2, 2-dioxido-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepin-9-yl]-1,3,4-oxadiazol-2-yl]-1-methyl-2-phenylethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

L9 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:365268 CAPLUS

DOCUMENT NUMBER: 144:412550

TITLE: Tricyclic indole derivatives for use in the treatment

of Alzheimer's disease

INVENTOR(S): Demont, Emmanuel Hubert; Redshaw, Sally; Walter, Daryl

Simon

PATENT ASSIGNEE(S): Glaxo Group Limited, UK PCT Int. Appl., 35 pp.

SOURCE:

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT	KIND DATE				APPL:	ICAT:	DATE											
WO 2006	TO 2006040148					20060420		1	WO 20	005-1		20051011						
W:	W: AE, AG, AL,																	
	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KP,	KR,	KZ,		
	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,		
	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,		
	SK,	SL,	SM,	SY,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,		
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	IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	BJ,		
	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,		
	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,		
	KG,	ΚZ,	MD,	RU,	ТJ,	TM												
PRIORITY APP	LN. I	NFO.	:		GB 2004-22755								A 20041013					
OTHER SOURCE	(S):			CASREACT 144:412550; MARPAT 144:412550														

OI GT

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The present invention relates to novel ketone compds. of formula I [R1 = H or C1-3 alkv1; R2 = C1-3 alkv1, C2-4 alkenv1, C2-4 alkvnv1, etc.; m = 0-4; n = 0-2; A-B = -NR5SO2-; R5 = H, C1-6 alkyl, C3-6 alkenyl, etc.; -W- = -CH2-, -(CH2)2-, -(CH2)3-, etc.; X-Y-Z = -NCR8=CR9-; R8 = H, C1-6 alkyl or C3-10 cycloalkyl; R9 = H, C1-6 alkyl, C1-6 alkoxy, etc.; R3 = C1-6 alkyl, C2-6 alkenvl, C2-6 alkvnvl, etc.; R4 = H, C1-10 alkvl, C3-10 alkenvl, etc. | having Asp2 (B-secretase, BACE1 or Memapsin-2) inhibitory activity, processes for their preparation, to compns, containing them and to

their use in the treatment of diseases characterized by elevated β -amyloid levels or β -amyloid deposits, particularly Alzheimer's disease.

((3S)-3-{[(7-ethyl-1-methyl-2,2-dioxido-3,4-dihydro-1H-

Thus, to a solution of 1,1-dimethylethyl

[1,2,5]thiadiazepino[3,4,5-hi]indol-9-yl)carbonyl]amino}-2-oxo-4phenylbutyl)tetrahydro-2H-pyran-4-ylcarbamate (II) in dioxane was added 4-methylbenzenesulfonic acid hydrate and the resulting mixture was stirred at rt for 16 h. The mixture was partitioned between Et acetate and a saturated

aqueous NaHCO3 solution The phases were separated and the organic phase was was washed,

dried and concentrated and the residue was purified by Mass Directed Autopreparation to give 7-ethyl-1-methyl-N-[(1S)-2-oxo-1-(phenylmethyl)-3-(tetrahydro-2H-pyran-4-ylamino)propyl]-3,4-dihydro-1H-[1,2,5]thiadiazepino(3,4,5-hi]indole-9-carboxamide 2,2-dioxide (III) in 35% yield. The exemplified compds. were tested in the Asp-2 inhibitory assay and the Cathepsin D inhibitory assay and exhibited inhibition < 10 uM in the Asp-2 inhibitory assay and > 10 fold selectivity for Asp2

over CatD. T 883726-66-7P 883726-67-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (USES)

(tricyclic indole derivs. for use in the treatment of diseases characterized by elevated $\beta\text{--amyloid}$ levels or $\beta\text{--amyloid}$ deposits, particularly Alzheimer's disease)

RN 883726-66-7 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, 7-ethyl-3,4-dihydro-1-methyl-N-[(1S)-2-oxo-1-(phenylmethyl)-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-,2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 883726-67-8 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, 7-ethyl-3,4-dihydro-N-[(1S)-3-[([3-methoxyphenyl]methyl]amino]-2-oxo-1-(phenylmethyl)propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

- IT 790252-03-8P 790252-31-2P 790254-39-6P 790254-40-9P 790254-64-7P 883726-62-3P 883726-63-4P 883726-63-4P 883726-64-5P 883726-65-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (tricyclic indole derivs. for use in the treatment of diseases
 - characterized by elevated β-amyloid levels or β-amyloid deposits, particularly Alzheimer's disease)
- RN 790252-03-8 CAPLUS
- CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide,
 7-ethyl-3,4-dihydro-N-[(15,2R)-2-hydroxy-3-[((3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]-1-methyl-, 2,2-dioxide
 (CA INDEX NAME)

Absolute stereochemistry.

- RN 790252-31-2 CAPLUS
- CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, 7-ethyl-3,4-dihydro-H[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-1-methyl-,2,2-dioxide (CA INDEX NAME)

- RN 790254-39-6 CAPLUS
- CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-40-9 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-methyl-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-64-7 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid,
7-ethyl-3,4-dihydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

RN 883726-62-3 CAPLUS

CN Carbamic acid, [(2R,3S)-3-[[(7-ethyl-3,4-dihydro-1-methyl-2,2-dioxido-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepin-9-yl)carbonyl]amino]-2-hydroxy-4-phenylbutyl](tetrahydro-2H-pyran-4-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 883726-63-4 CAPLUS

CN Carbamic acid, [(2R,3S)-3-[[(7-ethyl-3,4-dihydro-1-methyl-2,2-dioxido-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepin-9-yl)carbonyl]amino]-2-hydroxy-4-phenylbutyl][(3-methoxyphenyl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 883726-64-5 CAPLUS

CN Carbamic acid, [(3S)-3-[[(7-ethyl-3,4-dihydro-1-methyl-2,2-dioxido-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepin-9-yl)carbonyl]amino]-2-oxo-4-phenylbutyl](tetrahydro-2H-pyran-4-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 883726-65-6 CAPLUS

CN Carbamic acid, [(3S)-3-[[(7-ethyl-3,4-dihydro-1-methyl-2,2-dioxido-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepin-9-yl)carbonyl]amino]-2-oxo-4-phenylbutyl][(3-methoxyphenyl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

3

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:364095 CAPLUS

DOCUMENT NUMBER: 144:390951

TITLE: Heterocyclic ketone compounds for treating Alzheimer's

disease

INVENTOR(S): Demont, Emmanuel Hubert; Redshaw, Sally; Walter, Daryl

Simon

PATENT ASSIGNEE(S): Glaxo Group Ltd., UK

SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT NO.					KIN	D	DATE			APPL		DATE					
						-											
WO 2006040149				A1 20060420				WO 2	005-	EP11	002		20051011				
WO 2006040149			A9		2006	0824											
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		LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,
		NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,
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		CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
		GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
		KG.	KZ.	MD.	RU.	TJ.	TM										

PRIORITY APPLN. INFO.: GB 2004-22765 A 20041013
OTHER SOURCE(S): MARPAT 144:390951

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I [R1 = halogen or Cl-3 alkyl; R2 = Cl-3 alkyl, C2-4 alkenyl, C2-4 alkenyl, C2-4 alkenyl, C2-6 alkenyl, C3-6 alkenyl, etc.; m = 0-4; n = 0-2; A-B = -NRS502-; R5 = H, Cl-6 alkyl, C3-6 alkenyl, etc.; W = -CH2-, -(CH2)2-, -(CH2)3-, etc.; X-Y-Z = -C-CR8NR9-; R8 = H, Cl-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, etc.; K4 = H, Cl-10 alkyl, C3-10 alkenyl, c2-6 alkenyl, C2-6 alkynyl, etc.; R4 = H, Cl-10 alkyl, C3-10 alkenyl, etc.], having Asp2 (B-secretase, BACEI or Memapsin-2) inhibitory activity, are prepared and may be used in the treatment of diseases characterized by elevated β- amyloid levels or β-amyloid deposits, particularly Alzeimer's disease. Thus, compound II was Boc-protected with di-tert-butoxy dicarbonate and oxidized with Dess-Martin periodinane to provide III. Compound III was then Boc-deprotected to afford title compound IV-p-MeC6H4SO3H. Compound IV-p-MeC6H4SO3H was tested in the Asp-2 inhibitory assay and the Cathepsin D inhibitory assay and exhibited inhibition <10 μM in the Asp-2 inhibitory assay and >10 fold selectivity for Asp2 over CatD.

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of heterocyclic ketone compds, for the treatment of diseases characterized by elevated $\beta\text{-amyloid}$ levels or $\beta\text{-amyloid}$

deposits, particularly Alzheimer's disease)

RN 883565-28-4 CAPLUS CN Pvrrolo[4,3,2-ef]-2,

Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, 6-ethyl-1,3,4,6-tetrahydro-1-methyl-N-[(15)-2-oxo-1-(phenylmethyl)-3-

[(tetrahydro-2H-pyran-4-yl)amino]propyl]-, 2,2-dioxide, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 883565-27-3

CMF C29 H36 N4 O5 S

Absolute stereochemistry.

CM 2

CRN 104-15-4

CMF C7 H8 O3 S

IT 856696-25-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of heterocyclic ketone compds, for the treatment of diseases characterized by elevated β -amyloid levels or β -amyloid deposits, particularly Alzheimer's disease)

RN 856696-25-8 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide,

6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-1-methyl-,2,2-dioxide (CA INDEX NAME)

IT 883565-25-1P 883565-26-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heterocyclic ketone compds. for the treatment of diseases characterized by elevated $\beta\text{-amyloid}$ levels or $\beta\text{-amyloid}$ deposits, particularly Alzheimer's disease)

RN 883565-25-1 CAPLUS

CN Carbamic acid, [(2R,3S)-3-[[(6-ethyl-1,3,4,6-tetrahydro-1-methyl-2,2-dioxidopyrrolo[4,3,2-ef]-2,1-benzothiazepin-8-yl]carbonyl]amino]-2-hydroxy-4-phenylbutyl](tetrahydro-2H-pyran-4-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 883565-26-2 CAPLUS

CN Carbamic acid, [(3S)-3-[[(6-ethyl-1,3,4,6-tetrahydro-1-methyl-2,2-dioxidopyrrolo|4,3,2-ef]-2,1-benzothiazepin-8-yl)carbonyl]amino]-2-oxo-4-phenylbutyl](tetrahydro-2H-pyran-4-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

4

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:564675 CAPLUS

DOCUMENT NUMBER: 143:97337

TITLE: Preparation of tricyclic indole hydroxyethylamine

derivatives and their use in the treatment of

Alzheimer's disease

INVENTOR(S): Redshaw, Sally; Demont, Emmanuel Hubert; Walter, Daryl

Simon

PATENT ASSIGNEE(S): Glaxo Group Limited, UK SOURCE: PCT Int. Appl., 61 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

		KIND DATE															
WO	WO 2005058915 W: AE, AG, AL,					A1 20050630											
	₩:																
											, EC,						
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											, IT,						
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG	, CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,
		MR,	ΝE,	SN,	TD,												
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CA	2549	072			A1	2005	0630		CA:	2004-		20041209					
EP	1692	143			A1		2006	0823	EP 2004-803724						20041209		
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,					RO,	CY,	TR,	BG	, CZ,	EE,	HU,	PL,	SK,	HR,	IS
	1914				A		2007	0214		CN :	2004-		20041209				
BR	2004	A		2007	0508		BR :	2004-		20041209							
JP	2007	5139	13		T		2007	0531		JP :	2006-	5434	88		2	0041	209
IN	2006	DN02	954		Α						2006-						
US	2007	A1		2007	0329		US :	2006-		20060608							
MX	2006	PA06	572		A		2006	0731		MX :	2006-	PA65	72		2	0060	609
NO	2006	0031	37		A		2006	0831		NO :	2006-	3137			2	0060	706
PRIORIT	Y APP	LN.	INFO	. :						GB :	2003-	2890	0		A 2	0031	212
										WO :	2004-	EP14	076		W 2	0041	209
OTHER S	OURCE	(S):			CAS	REAC	T 14	3:97	337;	MA	RPAT	143:	9733	7			

OTHER SOURCE(S): CASREACT 143:97337; MARPAT 143:97337

$$(\mathbb{R}^1)_{\mathfrak{m}} \overset{\mathbb{R}^3}{\underset{\mathbb{V}}{\overset{\mathbb{R}^3}{\longrightarrow}}} \overset{\mathbb{R}^4}{\underset{\mathbb{V}}{\overset{\mathbb{R}^3}{\longrightarrow}}} \overset{\mathbb{R}^4}{\underset{\mathbb{V}}{\longrightarrow}} \overset{\mathbb{R}^4}{\overset{\mathbb{R}^4}{\longrightarrow}}$$

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AB The present invention relates to novel hydroxyethylamine compds. having Asp2 (B-secretase, BACE1 or Memapsin) inhibitory activity of formula I, processes for their preparation, to compns. containing them and to their use in

the treatment of diseases characterized by elevated B-amyloid levels or β-amyloid deposits, particularly Alzheimer's disease (no data). The variables for I are A-B = -NR5-SO2- or -NR5-CO-; R5 = H, alkyl, alkenyl, alkynyl, cycloalkyl, alkylaryl, alkyl-heteroaryl, alkyl-heterocyclyl, cycloalkyl-aryl or cycloalkyl-heteroaryl; -W- = -CH2-, -(CH2)2-, -(CH2)3-, -C(H)=C(H)- or -CH2-C(H)=C(H)-; X-Y-Z = -C=CR8-NR9-; R8 = H, C1-6 alkyl or C3-10 cycloalkyl; R9 = any group given for R5, COOR12a, OR12a, OONR12aR13a, SO2NR12aR13a, CO-alkyl, CO-rings, SO2-alkyl and -SO2-rings (wherein R12a and R13a independently represent H, C1-6 alkyl or C3-10 cycloalkyl); R3 = alkyl, alkenyl, alkynyl, alkyl-cycloalkyl, alkylaryl, alkylheteroaryl or alkylheterocyclyl; R4 = any group given for R3, other ring systems, C(RaRb), CONH-alkyl, C(RaRb)-CONH-alkyl/ring, alkyl-S-C alkyl, C2-6 alkyl-NRcRd, C(RaRb)-alkyl/ring, alkyl-O-alkylaryl/alkyl/ring; Ra and Rb independently = H. C1-6 alkyl or Ra and Rb together with the carbon atom to which they are attached may form a C3-10 cycloalkyl or heterocyclyl group; Rc and Rd independently = H, C1-6 alkyl, C3-10 cycloalkyl or Rc and Rd together with the nitrogen atom to which they are attached form a heterocyclyl group; or a pharmaceutically acceptable salt or solvate thereof. 856696-23-6P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-3-[[[3-(methyloxy)phenyl|methyl|amino|-1-(phenylmethyl)propyl|-1-methyl-1,3,4,6tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide 856696-25-8P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide 856696-29-2P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[[[1-(2,2,2-trifluoroethyl)-1H-pyrazol-4-yl]methyl]amino]propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate 856696-31-6P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmethyl)amino[propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate 856696-33-8P, 6-Ethvl-N-[(1S,2R)-2-hvdroxv-1-(phenvlmethvl)-3-[(4pyridinylmethyl)aminolpropyll-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate 856696-35-0P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(3pyridinylmethyl)amino[propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate 856696-37-2P 856696-38-3P, 6-Ethyl-N-[(1S,2R)-3-[[(3-ethyl-5-isoxazolyl)methyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3cd]indole-8-carboxamide 2,2-dioxide 856696-40-7P, N-[(1S, 2R)-3-(Cyclobutylamino)-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate 856696-42-9P, N-[(1S, 2R)-3-[(4, 4-Difluorocyclohexyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate 856696-44-1P, 6-Ethyl-N-[(1S,2R)-3-[(2-fluoroethyl)amino]-2hydroxy-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate

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856696-45-2P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-3-[(2,2,3,3,3-
pentafluoropropyl)aminol-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-
tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
856696-47-4P, 6-Ethyl-N-[(1S,2R)-3-[[(5-ethyl-3-
thienyl)methyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-
tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
formate 856696-49-6P, 6-Ethv1-N-|(1S,2R)-2-hvdroxy-3-||2-
(methyloxy)ethyllaminol-1-(phenylmethyl)propyll-1-methyl-1,3,4,6-
tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
formate 856696-50-9P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-1-
(phenylmethyl)-3-[(2,2,2-trifluoroethyl)amino]propyl]-1-methyl-1,3,4,6-
tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
856696-52-1P, 6-Ethvl-N-((1S,2R)-3-(ethvlamino)-2-hydroxy-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cd]indole-8-carboxamide 2,2-dioxide formate 856696-54-3P,
N-[(1S, 2R)-3-[(Cyclopropylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-
6-ethyl-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-
carboxamide 2,2-dioxide formate 856696-56-5P,
N-[(1S, 2R)-3-(Cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1-
methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide
2,2-dioxide formate 856696-58-7P,
N-[(1S,2R)-3-(3-Cyclopenten-1-ylamino)-2-hydroxy-1-(phenylmethyl)propyl]-6-
ethyl-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-
carboxamide 2.2-dioxide formate 856696-60-1P.
6-Ethyl-N-[(1S,2R)-3-[[2-(ethylthio)ethyl]amino]-2-hydroxy-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cdlindole-8-carboxamide 2,2-dioxide formate 856696-62-3P,
6-Ethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[[[3-
(trifluoromethyl)phenyl]methyl]amino]propyl]-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856696-64-5P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(1-
propylbutyl)amino]propyl]-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856696-66-7P, N-[(1S,2R)-3-[(4,4-Dimethylcyclohexyl)amino]-2-
hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856696-67-8P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-(2-
propyn-1-ylamino)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cdlindole-8-carboxamide 2,2-dioxide 856696-69-0P,
6-Ethvl-N-((1S, 2R)-2-hvdroxv-1-(phenylmethvl)-3-(2-propen-1-
vlamino)propvl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cd]indole-8-carboxamide 2,2-dioxide formate 856696-71-4P,
N-[(1S, 2R)-3-[(3, 3-Dimethylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-
6-ethyl-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-
carboxamide 2,2-dioxide formate 856696-73-6P,
6-Ethvl-N-((1S,2R)-2-hvdroxv-1-(phenvlmethvl)-3-((3,3,5,5-
tetramethylcyclohexyl)aminolpropyll-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856696-74-7P 856696-75-8P,
6-Ethyl-N-[(1S, 2R)-2-hydroxy-1-(phenylmethyl)-3-(propylamino)propyl]-1-
methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide
2,2-dioxide 856696-76-9P,
6-Ethyl-N-((1S,2R)-2-hydroxy-1-(phenylmethyl)-3-((3,3,3-
trifluoropropyl)amino[propyl]-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
856696-77-0P, N-[(1S,2R)-3-[(2,2-Difluoroethy1)amino]-2-hydroxy-1-
(phenylmethyl)propyl]-6-ethyl-1-methyl-1,3,4,6-tetrahydro-
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[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
856696-79-2P, 6-Ethvl-N-[(1S,2R)-3-[(2-ethvlbutvl)amino]-2-hvdroxv-
1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cd]indole-8-carboxamide 2,2-dioxide formate 856696-81-6P,
6-Ethyl-N-[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)amino]-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cdlindole-8-carboxamide 2,2-dioxide formate 856696-83-8P,
6-Ethyl-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(2,2,6,6-
tetramethylcyclohexyl)amino[propyl]-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856696-85-0P 856696-86-1P,
6-Ethyl-N-[(1S,2R)-2-hydroxy-3-[[2-(methylthio)ethyl]amino]-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cdlindole-8-carboxamide 2,2-dioxide 856696-87-2P
856696-89-4P, 6-Ethyl-N-[[(1S,2R)-2-hydroxy-3-[(2-methyl-2-propen-
1-y1) amino]-1-(phenylmethyl) propyl] methyl]-1, 3, 4, 6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856696-91-8P, N-[(1S,2R)-3-(3-Buten-1-ylamino)-2-hydroxy-1-
(phenylmethyl)propyl]-6-ethyl-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856696-92-9P, N-[(1S,2R)-3-(Cycloheptylamino)-2-hydroxy-1-
(phenylmethyl)propyl]-6-ethyl-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
856696-93-0P 856696-94-1P 856696-96-3P.
6-Ethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[[2-
(propyloxy)ethyllamino|propyll-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856696-98-5P, 6-Ethyl-N-[(1S,2R)-3-[(1-ethynylcyclohexyl)amino]-2-
hydroxy-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856696-99-6P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-3-[(4-
methylphenyl)amino]-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
856697-01-3P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-3-[(1-
methylcyclohexyl)amino]-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-
tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
formate 856697-03-5P,
6-Ethyl-N-[(1S,2R)-3-[(1-ethylcyclohexyl)amino]-2-hydroxy-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cdlindole-8-carboxamide 2,2-dioxide formate 856697-05-7P.
6-Ethvl-N-[(1S, 2R)-2-hydroxy-1-(phenylmethyl)-3-[(1-
propylcyclohexyl)amino[propyl]-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-07-9P, N-[(1S,2R)-3-[[2-[(1,1-
Dimethylethyl)thio|ethyl|amino|-2-hydroxy-1-(phenylmethyl)propyl|-6-ethyl-
1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide
2.2-dioxide formate 856697-09-1P.
6-Ethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[[2-[(2,2,2-
trifluoroethyl)oxy[ethyl]amino]propyl]-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-11-5P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-3-(phenylamino)-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cd]indole-8-carboxamide 2,2-dioxide formate 856697-13-7P,
6-Ethyl-N-[(1S, 2R)-2-hydroxy-3-[(3-methylphenyl)amino]-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cd]indole-8-carboxamide 2,2-dioxide formate 856697-15-9P,
6-Ethyl-N-[(1S,2R)-2-hydroxy-3-[(2-methylphenyl)amino]-1-
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(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cdlindole-8-carboxamide 2,2-dioxide formate 856697-17-1P,
6-Ethyl-N-[(1S,2R)-3-[[(1-ethyl-1H-pyrazol-4-yl)methyl]amino]-2-hydroxy-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cd]indole-8-carboxamide 2,2-dioxide formate 856697-19-3P,
6-Ethyl-N-[(1S,2R)-2-hydroxy-3-[(3-methyl-2-buten-1-yl)amino]-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cdlindole-8-carboxamide 2,2-dioxide formate 856697-21-7P.
6-Butvl-N-[(1S,2R)-3-(cvclohexylamino)-2-hvdroxy-1-(phenylmethyl)propyl]-1-
methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide
2,2-dioxide formate 856697-23-9P,
N-[(1S, 2R)-3-[(2-Chlorophenyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-6-
ethyl-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-
carboxamide 2,2-dioxide formate 856697-25-1P,
6-Ethyl-N-[(1S, 2R)-2-hydroxy-3-[[2-(methyloxy)phenyl]amino]-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cd]indole-8-carboxamide 2,2-dioxide formate 856697-27-3P,
6-Ethyl-N-[(1S, 2R)-2-hydroxy-3-[[4-(methyloxy)phenyl]amino]-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cdlindole-8-carboxamide 2,2-dioxide formate 856697-29-5P,
N-[(1S,2R)-3-[(3-Chlorophenyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-6-
ethyl-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-
carboxamide 2,2-dioxide formate 856697-31-9P,
6-Ethyl-N-[(1S, 2R)-2-hydroxy-3-[[3-(methyloxy)phenyl]amino]-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cdlindole-8-carboxamide 2,2-dioxide formate 856697-33-1P,
N-[(1S, 2R)-3-[(4-Chlorophenyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-6-
ethyl-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-
carboxamide 2,2-dioxide formate 856697-35-3P,
N-[(1S, 2R)-3-(Cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-1-methyl-
6-propyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide
2,2-dioxide formate 856697-37-5P,
N-[(1S, 2R)-3-(Cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-1-methyl-
6-(1-methylethyl)-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-
carboxamide 2,2-dioxide formate 856697-38-6P,
N-[(1S, 2R)-3-(Cyclopropylamino)-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-
1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide
2,2-dioxide 856697-40-0P,
N-[(1S, 2R)-2-Hydroxy-3-[[[3-(methyloxy)phenyl]methyl]amino]-1-
(phenylmethyl)propyl]-1-methyl-6-propyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-42-2P, N-[(1S,2R)-3-(Cyclohexylamino)-2-hydroxy-1-
(phenylmethyl)propyl]-1,6-diethyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cd]indole-8-carboxamide 2,2-dioxide formate 856697-44-4P,
N-[(1S, 2R)-3-[(2, 4-Dimethylphenyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-
6-ethyl-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-
carboxamide 2,2-dioxide formate 856697-46-6P.
N-[(1S, 2R)-3-[[4-(Dimethylamino)phenyl]amino]-2-hydroxy-1-
(phenylmethyl)propyl]-6-ethyl-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-48-8P, N-[(1S,2R)-3-(2-Butyn-1-ylamino)-2-hydroxy-1-
(phenylmethyl)propyl]-6-ethyl-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-50-2P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-
[(1,1,5-trimethylhexyl)amino]propyl]-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-52-4P, N-[(1S,2R)-3-(Butylamino)-2-hydroxy-1-
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(phenylmethyl)propyl]-6-ethyl-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-54-6P, N-[(1S,2R)-3-[[2,3-Bis(methyloxy)phenyl]amino]-2-
hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-56-8P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[[[3-
[(trifluoromethv1)oxv]phenv1|methv1|amino|propv1|-1-methv1-1,3,4,6-
tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
formate 856697-58-0P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-3-[[(6-methyl-
2-pyridinyl)methyl]amino]-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-
tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
formate 856697-60-4P 856697-62-6P,
6-Ethyl-N-[(1S, 2R)-2-hydroxy-3-[((1R)-1-methylpropyl)amino]-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cd]indole-8-carboxamide 2,2-dioxide formate 856697-64-8P,
6-Ethyl-N-[(1S, 2R)-2-hydroxy-3-[((1S)-1-methylpropyl)amino]-1-
(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-
cd]indole-8-carboxamide 2,2-dioxide formate 856697-66-0P,
6-Ethyl-N-((1S, 2R)-2-hydroxy-1-(phenylmethyl)-3-((2-
pyridinylmethyl)aminolpropyll-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-68-2P, 6-Ethv1-N-((1S,2R)-2-hvdroxy-3-((2-methv1-4-
(methyloxy)phenyl]amino]-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-
tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
formate 856697-70-6P, 6-Ethvl-N-((1S,2R)-3-((1-
ethylcyclopropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-
tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
formate 856697-72-8P, 6-Ethyl-N-I(1S,2R)-2-hydroxy-3-(2-pentyn-1-
ylamino)-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-74-0P, 6-Ethyl-N-[(1S,2R)-3-[(3-fluoropropyl)amino]-2-
hydroxy-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-75-1P, 6-Ethyl-N-[(1S,2R)-2-hydroxy-3-[(1-
methylcyclopropyl)amino]-1-(phenylmethyl)propyl]-1-methyl-1,3,4,6-
tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide
856697-76-2P, 1,6-Diethyl-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-
[(tetrahydro-2H-pyran-4-v1)amino[propyl]-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
856697-78-4P, N-[(1S,2R)-3-[(1,1-Dimethyl-2-propyn-1-yl)amino]-2-
hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide formate
856697-79-5P, N-[(1S,2R)-3-(Cyclooctylamino)-2-hydroxy-1-
(phenylmethyl)propyl]-6-ethyl-1-methyl-1,3,4,6-tetrahydro-
[1,2]thiazepino[5,4,3-cd]indole-8-carboxamide 2,2-dioxide
857052-39-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (drug candidate; preparation of tricyclic indole hydroxyethylamine derivs.
   and their use in treatment of Alzheimer's disease)
856696-23-6 CAPLUS
Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide,
6-ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-[[(3-
```

methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]-1-methyl-, 2,2-dioxide

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(CA INDEX NAME)

RN

CN

Absolute stereochemistry.

- RN 856696-25-8 CAPLUS
- CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,ZR)-2-hydroxy-1-(phenylmethyl)-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-1-methyl-,2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

- RN 856696-29-2 CAPLUS
- CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[[[1-(2,2,2-trifluoroethyl)-1H-pyrazol-4yl]methyl]amino]propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)
 - CM

1

- CRN 856696-28-1
- CMF C30 H35 F3 N6 O4 S

CM

CRN 64-18-6 CMF C H2 O2

о == сн - он

 $856696-31-6 \quad CAPLUS \\ Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3--[(phenylm$ 2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 856696-30-5 CMF C31 H36 N4 O4 S

Absolute stereochemistry.

CM 2

О== СН-ОН

RN 856696-33-8 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(4-pyridinylmethyl) amino]propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-32-7 CMF C30 H35 N5 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 856696-35-0 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,28)-2-hydroxy-1-(phenylmethyl)-3-[(3-pyridinylmethyl) amino]propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-B-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-34-9 CMF C30 H35 N5 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн - он

CN methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 856696-36-1

CMF C31 H42 N4 O5 S

Absolute stereochemistry.

CM

O CH OH

RN 856696-38-3 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide,
6-ethyl-N-[(18,2R)-3-[[(3-ethyl-5-isoxazolyl)methyl]amino]-2-hydroxy-1(phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methyl-,2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 856696-40-7 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-(cyclobutylamino)-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrol(4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-39-4 CMF C28 H36 N4 O4 S

Absolute stereochemistry.

CM 2

О== СН- ОН

RN 856696-42-9 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-[(4,4-difluorocyclohexyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 856696-41-8 CMF C30 H38 F2 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн− он

RN 856696-44-1 CAPLUS

CN Formic acid, compd. with 6-ethyl-N-[(1S,2R)-3-[(2-fluoroethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazebine-8-carboxamide 2,2-dioxide (1:1) (CA NNDEX NAME)

CM 1

CRN 856696-43-0 CMF C26 H33 F N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН-ОН

 $856696-45-2 \quad {\tt CAPLUS} \\ {\tt Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide,} \\$ CN 6-ethyl-1, 3, 4, 6-tetrahydro-N-[(1S, 2R)-2-hydroxy-3-[(2, 2, 3, 3, 3pentafluoropropyl)amino]-1-(phenylmethyl)propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 856696-47-4 CAPLUS

Formic acid, compd. with 6-ethyl-N-[(1S,2R)-3-[[(5-ethyl-3thieny1)methy1]amino]-2-hydroxy-1-(pheny1methy1)propy1]-1,3,4,6-tetrahydro-1-methy1pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-46-3 CMF C31 H38 N4 O4 S2

Absolute stereochemistry.

CN

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн - он

RN 856696-49-6 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-3-[(2-methoxyethyl)amino]-1-(phenylmethyl)propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-48-5 CMF C27 H36 N4 O5 S

Absolute stereochemistry.

CM 2

О== СН- ОН

RN 856696-50-9 CAPLUS

Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, CN 6-ethv1-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(2,2,2trifluoroethyl)amino]propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

856696-52-1 CAPLUS Formic acid, compd. with 6-ethyl-N-[(lS,2R)-3-(ethylamino)-2-hydroxy-1-CN (phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-51-0 CMF C26 H34 N4 O4 S

Absolute stereochemistry.

CM 2

О== СН- ОН

RN 856696-54-3 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-[(cyclopropylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-53-2 CMF C28 H36 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 856696-56-5 CAPLUS

CN Formic acid, compd. with N={(15,2R)-3-(cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-55-4 CMF C30 H40 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн - он

856696-58-7 CAPLUS Formic acid, compd. with N-[(1S,2R)-3-(3-cyclopenten-1-ylamino)-2-hydroxy-CN 1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-57-6 CMF C29 H36 N4 O4 S

Absolute stereochemistry.

CM 2

О== СН- ОН

RN 856696-60-1 CAPLUS

CN Formic acid, compd. with 6-ethyl-N-[(1S,2R)-3-[[2-(ethylthio)ethyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM I

CRN 856696-59-8

CMF C28 H38 N4 O4 S2

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН-ОН

RN 856696-62-3 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[[[3-(trifluoromethyl)phenyl]methyl]amino]propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-61-2 CMF C32 H35 F3 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн - он

 $856696-64-5 \quad \text{CAPLUS} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-model)} \\ \text{CAPLUS} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-model)} \\ \text{CAPLUS} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-model)} \\ \text{CAPLUS} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-model)} \\ \text{CAPLUS} \\ \text{CAPLUS}$ (phenylmethyl)-3-[(1-propylbutyl)amino]propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-63-4 CMF C31 H44 N4 O4 S

Absolute stereochemistry.

CM 2

О== СН- ОН

RN 856696-66-7 CAPLUS

CN Formic acid, compd. with N={(18,2R)-3-[(4,4-dimethylcyclohexyl)maino]-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (i:1) (CA INBEN NAME)

CM 1

CRN 856696-65-6 CMF C32 H44 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн− он

RN 856696-67-8 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-(2-propyn-1-ylamino)propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

RN 856696-69-0 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-(2-propen-1-ylamino)propyl)-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM :

CRN 856696-68-9 CMF C27 H34 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 856696-71-4 CAPLUS

CN Formic acid, compd with N=[(1S,2R)-3-[(3,3-dimethylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl)-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 856696-70-3

CMF C30 H42 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 856696-73-6 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(3,3,5,5-tetramethylcyclohexyl)amino|propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide

(1:1) (CA INDEX NAME)

CM 1

CRN 856696-72-5 CMF C34 H48 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

O == CH = OH

RN 856696-74-7 CAPLUS

Absolute stereochemistry.

- RN 856696-75-8 CAPLUS
- CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-(propylamino)propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

- RN 856696-76-9 CAPLUS
- CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, 6-ethyl-1,3,4,6-tetrahydro-N-[(18,2R)-2-hydroxy-1-(phenylmethyl)-3-[(3,3,3-trifluoropropyl)amino]propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

RN 856696-77-0 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide,
N=[(15,2R)-3-[(2,2-difluoroethyl)]amino]-2-hydroxy-1-(phenylmethyl)propyl]6-ethyl-1,3,4,6-tetrahydro-1-methyl-,2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 856696-79-2 CAPLUS

CN Formic acid, compd. with 6-ethyl-N-[(1S,2R)-3-[(2-ethylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 856696-78-1 CMF C30 H42 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн - он

 $856696-81-6 \quad \text{CAPLUS} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-model)} \\ \text{Capture} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-model)} \\ \text{Capture} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-model)} \\ \text{Capture} \\ \text{C$ CN [(3-methylbutyl)amino]-1-(phenylmethyl)propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-80-5 CMF C29 H40 N4 O4 S

Absolute stereochemistry.

CM 2

O CH OH

RN 856696-83-8 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,78],-2-hydroxy-1-(phenylmethyl)-3-[(2,2,6,6-tetramethylcyclohexyl)aminol propyl]-1 methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INBEN NAME)

CM 1

CRN 856696-82-7 CMF C34 H48 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн− он

RN 856696-85-0 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-[(2,2-dimethylcyclohexyl)amino]-2-hydroxy-1-(phenylmethylpropyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-84-9 CMF C32 H44 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН- ОН

RN 856696-86-1 CAPLUS

No. 1 Computer Service of the Computer of the

Absolute stereochemistry.

RN 856696-87-2 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, N-[(15,2R)-3-[(2-cyclohexylethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

RN 856696-89-4 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-3-[(2-methyl-2-propen-1-yl) amino]-1-(phenylmethyl)propyl]-1methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 856696-88-3 CMF C28 H36 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН-ОН

RN 856696-91-8 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-(3-buten-1-ylamino)-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856696-90-7 CMF C28 H36 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн− он

RN 856696-92-9 CAPLUS

Absolute stereochemistry.

RN 856696-93-0 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-(tricyclo[3.3.1.13,7]dec-2-ylamino)propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

RN 856696-94-1 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide,
N-[(15,2R)-3-[(1R,48)-bicyclo[2.2.1]hept-2-ylamino]-2-hydroxy-1(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methyl-, 2,2-dioxide
(CA INDEX NAME)

Absolute stereochemistry.

RN 856696-96-3 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(2-propoxyethyl)amino]propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAE)

CM 1

CRN 856696-95-2

CMF C29 H40 N4 O5 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн - он

 $856696-98-5 \quad \text{CAPLUS} \\ \text{Formic acid, compd. with } 6-\text{ethyl-N-[(1S,2R)-3-[(1-\text{ethynylcyclohexyl)amino]-}} \\ \\$ 2-hydroxy-1-(phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 856696-97-4 CMF C32 H40 N4 O4 S

Absolute stereochemistry.

CM 2

О== СН- ОН

RN 856696-99-6 CAPLUS

Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, CN 6-ethv1-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-[(4-methv1phenyl)amino]-1-(phenylmethyl)propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

856697-01-3 CAPLUS Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-CN [(1-methylcyclohexyl)amino]-1-(phenylmethyl)propyl]-1-methylpyrrolo[4,3,2ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 856697-00-2 CMF C31 H42 N4 O4 S

Absolute stereochemistry.

CM 2

RN 856697-03-5 CAPLUS

CN Formic acid, compd. with 6-ethyl-N-[(1S,2R)-3-[(1-ethylcyclohexyl)amino]-2hydroxy-1-(phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-02-4 CMF C32 H44 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 856697-05-7 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(1-propylcyclohexyl)amino]propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-04-6 CMF C33 H46 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн − он

856697-07-9 CAPLUS Formic acid, compd. with N-[(1S,2R)-3-[[2-[(1,1-CN dimethylethyl)thio]ethyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-06-8

CMF C30 H42 N4 O4 S2

Absolute stereochemistry.

2 CM

CRN 64-18-6

CMF C H2 O2

о СН-ОН

RN 856697-09-1 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(2-(2,2,2-trifluoroethoxy)tethyl]aminojpropyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM I

CRN 856697-08-0

CMF C28 H35 F3 N4 O5 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 856697-11-5 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-3-(phenylamino)-1-(phenylmethyl)propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-10-4 CMF C30 H34 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн − он

 $856697-13-7 \quad \text{CAPLUS} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-hydroxy$ [(3-methylphenyl)amino]-1-(phenylmethyl)propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-12-6 CMF C31 H36 N4 O4 S

Absolute stereochemistry.

CM 2

RN 856697-15-9 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,28)-2-hydroxy-3-[(2-methylphenyl) amino]-1-(phenylmethyl) propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-cazboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-14-8 CMF C31 H36 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 856697-17-1 CAPLUS

CN Formic acid, compd. with 6-ethyl-N-[(15,2R)-3-[[(1-ethyl-1H-pyrazol-4-yl)methyl]mino]-2-hydroxy-1-(phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-16-0 CMF C30 H38 N6 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн − он

 $856697-19-3 \quad CAPLUS \\ Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-[(3-methyl-2-buten-1-yl)lamino]-1-(phenylmethyl)propyl]-1$ methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-18-2 CMF C29 H38 N4 O4 S

Absolute stereochemistry.

2 CM

о--- сн-- он

RN 856697-21-7 CAPLUS

CN Formic acid, compd. with 6-butyl-N-[(1S,2R)-3-(cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-20-6 CMF C32 H44 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн− он

RN 856697-23-9 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-[(2-chlorophenyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-22-8 CMF C30 H33 C1 N4 O4 S

CHE C30 H33 CI N4 04 5

CM

CRN 64-18-6 CMF C H2 O2

о == сн − он

 $856697-25-1 \quad \text{CAPLUS} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-model)} \\ \text{Capture} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-model)} \\ \text{Capture} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-model)} \\ \text{Capture} \\ \text{C$ CN [(2-methoxyphenyl)amino]-1-(phenylmethyl)propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-24-0 CMF C31 H36 N4 O5 S

Absolute stereochemistry.

CM 2

RN 856697-27-3 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-[(4-methoxyphenyl)amino]-1-(phenylmethyl)propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-26-2 CMF C31 H36 N4 O5 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 856697-29-5 CAPLUS

CN Formic acid, compd. with N={(1S,2R)-3-{(3-chlorophenyl)amino}-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAVE)

CM 1

CRN 856697-28-4

CMF C30 H33 C1 N4 O4 S

CM

CRN 64-18-6 CMF C H2 O2

о == сн − он

[(3-methoxyphenyl)amino]-1-(phenylmethyl)propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-30-8 CMF C31 H36 N4 O5 S

Absolute stereochemistry.

CM 2

RN 856697-33-1 CAPLUS

CN Formic acid, compd. with N-[(15,2R)-3-[(4-chlorophenyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-32-0

CMF C30 H33 C1 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

o== cн- он

RN 856697-35-3 CAPLUS

CN Formic acid, compd. with N={(15,28)-3-(cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methyl-6-propylpyrrolo{4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-34-2

CMF C31 H42 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн − он

856697-37-5 CAPLUS Formic acid, compd. with N-[(1S,2R)-3-(cyclohexylamino)-2-hydroxy-1-CN (phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methyl-6-(1-methylethyl)pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-36-4 CMF C31 H42 N4 O4 S

Absolute stereochemistry.

2 CM

о--- сн-- он

RN 856697-38-6 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, N-[(1S,2R)-3-(cyclopropylamino)-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 856697-40-0 CAPLUS

CN Formic acid, compd. with 1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]-1-methyl-6-propylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-39-7 CMF C33 H40 N4 O5 S

Absolute stereochemistry.

CM 2

RN 856697-42-2 CAPLUS

CN Formic acid, compd. with N-{(18,2R)-3-(cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-1,6-diethyl-1,3,4,6-tetrahydropyrrolo[4,3,2-ef]-2,1benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-41-1 CMF C31 H42 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 856697-44-4 CAPLUS

CN Formic acid, compd. with N=[(15,2R)-3-[(2,4-dimethylphenyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-43-3 CMF C32 H38 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн − он

RN 856697-46-6 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-[[4-(dimethylamino)phenyl]amino]-2hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-45-5 CMF C32 H39 N5 O4 S

Absolute stereochemistry.

CM 2

RN 856697-48-8 CAPLUS

CN Formic acid, compd. with N-[(15,2R)-3-(2-butyn-1-ylamino)-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-47-7 CMF C28 H34 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН-ОН

RN 856697-50-2 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(1,1,5-trimethylhexyl)aminolpropyl]-1 methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (i:1) (CA INDEX NAME)

CM 1

CRN 856697-49-9 CMF C33 H48 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн − он

CN

856697-52-4 CAPLUS Formic acid, compd. with N-[(1S,2R)-3-(butylamino)-2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-51-3 CMF C28 H38 N4 O4 S

Absolute stereochemistry.

CM 2

RN 856697-54-6 CAPLUS

CN Formic acid, compd. with N=[(15,2R)-3-[(2,3-dimethoxyphenyl)amino]-2hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 856697-53-5 CMF C32 H38 N4 O6 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН= ОН

RN 856697-56-8 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[[[3-(trifluoromethoxy)phenyl]methyl]amino]propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-55-7

CMF C32 H35 F3 N4 O5 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн − он

 $856697-58-0 \quad CAPLUS \\ Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-[(16-methyl-2-pyridinyl)methyl]amino]-1-(phenylmethyl)propyl]-1$ methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-57-9 CMF C31 H37 N5 O4 S

Absolute stereochemistry.

2 CM

о--- сн-- он

RN 856697-60-4 CAPLUS

CN Formic acid, compd. with N-[(1S, 2R)-3-[[2-(cyclohexylamino)-1-methyl-2-oxoethyl]amino]-2-hydroxy-1-(phenylmethyl)propy]1-6-ethyl-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-59-1

CMF C33 H45 N5 O5 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 856697-62-6 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-3[[(1R)-1-methylpropyl]amino]-1-(phenylmethyl)propyl]-1-methylpyrrolof(4,3,2ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-61-5

CMF C28 H38 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн - он

 $856697-64-8 \quad \text{CAPLUS} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-model)} \\ \text{Capture} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-model)} \\ \text{Capture} \\ \text{Formic acid, compd. with } 6-\text{ethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-3-model)} \\ \text{Capture} \\ \text{C$ [[(1S)-1-methylpropyl]amino]-1-(phenylmethyl)propyl]-1-methylpyrrolo[4,3,2ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-63-7 CMF C28 H38 N4 O4 S

Absolute stereochemistry.

CM 2

RN 856697-66-0 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,28]-2-hydroxy-1-(phenylmethyl)-3-[(2-pyridinylmethyl)amino]propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-65-9 CMF C30 H35 N5 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

o== cн- он

RN 856697-68-2 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,2R)-2-hydroxy-3-[(4-methoxy-2-methylphenyl) amino]-1-(phenylmethyl) propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-67-1 CMF C32 H38 N4 O5 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн - он

856697-70-6 CAPLUS Formic acid, compd. with 6-ethyl-N-[(1S,2R)-3-[(1-ethylcyclopropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-69-3 CMF C29 H38 N4 O4 S

Absolute stereochemistry.

CM 2

RN 856697-72-8 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(15,28]-2-hydroxy-3-(2-pentyn-1-ylamino)-1-(phenylmethyl)propyl]-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-71-7

CMF C29 H36 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн - он

RN 856697-74-0 CAPLUS

CN Formic acid, compd. with 6-ethyl-N-[(15,2R)-3-[(3-fluoropropy)]amino]-2-hydroxy-1-(phenylmethyl)propyl]-1,3,4,6-tetrahydro-1-methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 856697-73-9

CMF C27 H35 F N4 O4 S

CRN 64-18-6 CMF C H2 O2

О== СН-ОН

856697-75-1 CAPLUS
Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, CN 6-ethyl-1, 3, 4, 6-tetrahydro-N-[(1S, 2R)-2-hydroxy-3-[(1methylcyclopropyl)amino]-1-(phenylmethyl)propyl]-1-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 856697-76-2 CAPLUS CN

Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide, 1,6-diethyl-1,3,4,6-tetrahydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-, 2,2-dioxide (CA INDEX NAME)

RN 856697-78-4 CAPLUS

CN Formic acid, compd. with N-[(18,2R)-3-[(1,1-dimethyl-2-propyn-1-y1)amino]2-hydroxy-1-(phenylmethyl)propyl]-6-ethyl-1,3,4,6-tetrahydro-1methylpyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide 2,2-dioxide
(1:1) (CA INDEX NAME)

CM :

CRN 856697-77-3 CMF C29 H36 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН-ОН

RN 856697-79-5 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxamide,
N-[(15,2R)-3-(cyclooctylamino)-2-hydroxy-1-(phenylamethyl)propyl]-6-ethyl1,3,4,6-tetrahydro-1-methyl-,2,2-dioxide (CA INDEX NAME)

RN 857052-39-2 CAPLUS

CN Formic acid, compd. with 6-ethyl-1,3,4,6-tetrahydro-N-[(18,2R)-2-hydroxy-3-[(14-methylcyclohexyl)amino]-1-(phenylmethyl)propyl]-1-methylpyrrolo[4,3,2-4]-2,1-benzothiazepin-8-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM :

CRN 857052-38-1

CMF C31 H42 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН- ОН

IT 856695-82-4P 856695-95-9P 856695-96-0P,
6-Ethyl-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxylic acid 2,2-dioxide 856696-02-1P,
1-Methyl-6-(1-methylethyl)-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxylic acid 2,2-dioxide 856696-03-2P,
1-Methyl-6-propyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxylic acid 2,2-dioxide 856696-03-2P,
6-Butyl-1-methyl-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-carboxylic acid 2,2-dioxide 856696-05-4P,

1,6-Diethy1-1,3,4,6-tetrahydro-[1,2]thiazepino[5,4,3-cd]indole-8-

carboxylic acid 2,2-dioxide

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tricyclic indole hydroxyethylamine derivs. and their use in treatment of Alzheimer's disease)

RN 856695-82-4 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxylic acid,

1,3,4,6-tetrahydro-1-methyl-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 856695-95-9 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxylic acid, 6-ethyl-1,3,4,6-tetrahydro-1-methyl-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 856695-96-0 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxylic acid, 6-ethyl-1,3,4,6-tetrahydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

RN 856696-02-1 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxylic acid, 1,3,4,6-tetrahydro-1-methyl-6-(1-methylethyl)-, 2,2-dioxide (CA INDEX NAME)

RN 856696-03-2 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxylic acid, 1,3,4,6-tetrahydro-1-methyl-6-propyl-, 2,2-dioxide (CA INDEX NAME)

RN 856696-04-3 CAPLUS

CN Pyrrolo[4,3,2-ef]-2,1-benzothiazepine-8-carboxylic acid,
6-butyl-1,3,4,6-tetrahydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

RN 856696-05-4 CAPLUS CN Pyrrolo(4,3,2-ef]-2,1-benzothiazepine-8-carboxylic acid, 1,5-diethyl-1,3,4,6-tetrahydro-, 2,2-dioxide (CA INDEX NAME)

REFERENCE COUNT:

9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L9 ANSWER 5 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:927212 CAPLUS

DOCUMENT NUMBER: 141:395588

TITLE: Preparation of hydroxydiaminopropyl tricyclic indolecarboxamides for treatment of β -amyloid

related disease.

INVENTOR(S): Demont, Emmanuel Hubert; Redshaw, Sally; Walter, Daryl

Simon
PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 74 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.			APPLICATION NO.	
			WO 2004-EP4244	
			BA, BB, BG, BR, BW,	
			DM, DZ, EC, EE, EG,	
			IN, IS, JP, KE, KG,	
			MD, MG, MK, MN, MW,	
			RO, RU, SC, SD, SE,	
			UG, US, UZ, VC, VN,	
			SD, SL, SZ, TZ, UG,	
			AT, BE, BG, CH, CY,	
			IT, LU, MC, NL, PL,	
	BF, BJ, CF	f, CG, C1,	CM, GA, GN, GQ, GW,	ML, MR, NE, SN,
TD, TG	3.1	20041104	AU 2004-232475	20040421
			CA 2004-2523291	
			EP 2004-728567	
			GB, GR, IT, LI, LU,	
			TR, BG, CZ, EE, HU,	
CN 1000572	n n	20060416	BR 2004-9622 CN 2004-80017561 JP 2006-505223	20040421
TD 2006524206	T	20061026	TD 2006-505223	20040421
TN 2005DN04531	Δ.	20001020	IN 2005-DN4531	20051006
IIS 2005DR04331	7.1	20070017	US 2005-553878	20051000
			NO 2005-5442	
PRIORITY APPLN. INFO		2000111	GB 2003-9221	
			WO 2004-EP4244	
OTHER SOURCE(S):	MARPAI	T 141:39558		

Т

$$(\mathbb{R}^1)_{\mathfrak{m}} \underbrace{\overset{B}{\underset{Y-Z}{\overset{A}{\longrightarrow}}}}_{H} \underbrace{\overset{N}{\underset{H}{\overset{N}{\longrightarrow}}}}_{OH} \underbrace{\overset{NHR}{^4}}$$

Page 323

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AR
    Title compds.[I; R1, R2 = alkyl, alkenyl, halo, alkoxy, amino, cyano, OH;
    m, n = 0-2; p = 1, 2; AB = NR5SO2, NR5CO; R5 = H, alky1, alkeny1, alkyny1,
     cycloalkyl, aryl, heteroaryl, aralkyl, heteroaralkyl, arylcycloalkyl,
     heteroarylcycloalkyl; XYZ = NCR8:CR9; R8 = H, alkyl, cycloalkyl; R9 = R8,
     aryl, heteroaryl, aralkyl, heteroarylalkyl, etc.; R3 = (substituted)
     alkyl, alkenyl, alkynyl, alkylcycloalkyl, alkylaryl, alkylheteroaryl,
     alkylheterocyclyl; R4 = H, (substituted) alkyl, alkynyl, cycloalkyl,
     cycloalkenyl, aryl, heteroaryl, heterocyclyl, alkylcycloalkyl,
     cycloalkylaryl, heterocyclylaryl, etc.], were prepared Thus,
     7-ethyl-2-oxo-1,2,3,4-tetrahydro[1,4]diazepino[3,2,1-hi]indole-9-
     carboxylic acid (preparation given),
(2R, 3S)-3-amino-1-(3-methoxybenzylamino)-4-
     phenylbutan-2-ol ditosylate, 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide
     hydrochloride, 1-hydroxybenzotriazole hydrate, and 4-ethylmorpholine were
     stirred 4 h in CH2C12/DMF to give 7-ethyl-2-oxo-1,2,3,4-
     tetrahydro[1,4]diazepino[3,2,1-hi]indole-9-carboxylic acid
     [(1S, 2R)-1-benzyl-2-hydroxy-3-(3-methoxybenzylamino)propyl]amide. I
     inhibited Asp-2 with IC50 <10 µM.
     790252-02-7P 790252-03-8P 790252-04-9P
     790252-06-1P 790252-08-3P 790252-10-7P
     790252-12-9P 790252-14-1P 790252-16-3P
     790252-18-5P 790252-20-9P 790252-22-1P
     790252-24-3P 790252-26-5P 790252-28-7P
790252-30-1P 790252-32-3P 790252-34-5P
     790252-36-7P 790252-38-9P 790252-40-3P
     790252-42-5P 790252-44-7P 790252-46-9P
     790252-48-1P 790252-50-5P 790252-52-7P
     790252-54-9P 790252-56-1P 790252-58-3P
     790252-60-7P 790252-62-9P 790252-64-1P
     790252-66-3P 790252-68-5P 790252-70-9P
     790252-72-1P 790252-74-3P 790252-75-4P
     790252-77-6P 790252-78-7P 790252-79-8P
     790252-81-2P 790252-83-4P 790252-85-6P
     790252-87-8P 790252-89-0P 790252-91-4P
     790252-93-6P 790252-96-9P 790252-99-2P
     790253-02-0P 790253-05-3P 790253-08-6P
     790253-11-1P 790253-13-3P 790253-15-5P
     790253-17-7P 790253-19-9P 790253-21-3P
     790253-23-5P 790253-26-8P 790253-29-1P
     790253-32-6P 790253-35-9P 790253-37-1P
     790253-39-3P 790253-41-7P 790253-43-9P
     790253-45-1P 790253-47-3P 790253-49-5P
     790253-51-9P 790253-85-9P 790253-87-1P
     790253-89-3P 790253-91-7P 790253-93-9P
     790253-95-1P 790253-97-3P 790253-99-5P
     790254-01-2P 790254-03-4P 790254-05-6P
     790254-07-8P 790254-09-0P 790254-11-4P
     790254-12-5P 790254-13-6P 790254-15-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of hydroxydiaminopropyl tricyclic indolecarboxamides for
        treatment of B-amyloid related disease)
RN
     790252-02-7 CAPLUS
CN
     1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide,
     7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[(3-
```

methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 790252-03-8 CAPLUS

CN 1H-Pyrrolo(1,2,3-ef)-2,1,5-benzothiadiazepine-9-carboxamide,
7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[((3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]-1-methyl-, 2,2-dioxide
(CA INDEX NAME)

Absolute stereochemistry.

RN 790252-04-9 CAPLUS

RN 790252-06-1 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[[[3-(trifluoromethyl)phenyl]methyl]amino]propyl]-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM :

CRN 790252-05-0 CMF C32 H35 F3 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН-ОН

RN 790252-08-3 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[[(3-(trifluoromethyl)phenyl]methyl]amino]propyl]-1,3-dimethyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-07-2 CMF C33 H37 F3 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN

790252-10-7 CAPLUS Formic acid, compd. with N-[(1\$,2\$)-3-(cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME) CN

CM

CRN 790252-09-4

CMF C30 H40 N4 O4 S

Absolute stereochemistry.

CM

CRN 64-18-6 CMF C H2 O2

O== CH- OH

RN 790252-12-9 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-(cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1,3-dimethyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM :

CRN 790252-11-8 CMF C31 H42 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

o== сн- он

RN 790252-14-1 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[(1,1,5-trimethylhexyl)amino]propyl]-1,3-dimethyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-13-0 CMF C34 H50 N4 O4 S

CRN 64-18-6 CMF C H2 O2

о == сн-он

790252-16-3 CAPLUS Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(1,1,5-trimethylhexyl)amino]propyl]-1-methyl-lH-CN pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-15-2 CMF C33 H48 N4 O4 S

Absolute stereochemistry.

CM 2

О СН ОН

RN 790252-18-5 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[1methyl-1-[3-(trifluoromethyl)phenyl]ethyl]amino]-1-(phenylmethyl)propyl]-1methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-17-4 CMF C34 H39 F3 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН-ОН

RN 790252-20-9 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1 (phenylmethyl)-3-[[[3-(trifluoromethyl)phenyl]methyl]amino]propyl]-1 (phenylmethyl)-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide
 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-19-6 CMF C38 H39 F3 N4 O4 S

CRN 64-18-6 CMF C H2 O2

о == сн-он

 $790252-22-1 \quad CAPLUS \\ \mbox{Formic acid, compd. with } 7-\mbox{ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[1-(3-R)-2-hydroxy-3-[1-(3-$ CN methoxyphenyl)-1-methylethyl]amino]-1-(phenylmethyl)propyl]-1,3-dimethyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide
(1:1) (CA INDEX NAME)

CM 1

CRN 790252-21-0 CMF C35 H44 N4 O5 S

Absolute stereochemistry.

CM 2

О СН ОН

RN 790252-24-3 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(15,2R)-2-hydroxy-3-[[1-(3-methoxyphenyl)-1-methylethyl]amino]-1-(phenylmethyl)propyl-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-23-2 CMF C34 H42 N4 O5 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790252-26-5 CAPLUS

CN Formic acid, compd. with 7-ethyl-N-[(15,2R)-3-[[(1-ethyl-1H-pyrazol-4-y1)methyl]maino]-2-hydroxy-1-(phenylmethyl)propyl]-3,4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-25-4 CMF C30 H38 N6 O4 S

CRN 64-18-6 CMF C H2 O2

о == сн - он

790252-28-7 CAPLUS Formic acid, compd. with 7-ethyl-N-[(lS,2R)-3-[[(1-ethyl-lH-pyrazol-4- $^{\prime\prime}]$ CN yl)methyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-3,4-dihydro-1,3dimethyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-27-6 CMF C31 H40 N6 O4 S

Absolute stereochemistry.

CM

О— СН— ОН

RN 790252-30-1 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-M-[(15,2R)-2-hydroxy-3-{(1-methylethyl)amino]-1-(phenylmethyl)propyl]-1-methyl-1H-pyrrolo[1,2,3-et]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-29-8 CMF C27 H36 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790252-32-3 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-31-2 CMF C29 H38 N4 O5 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн-он

790252-34-5 CAPLUS Formic acid, compd. with N-[(1S,2R)-3-(cyclopropylamino)-2-hydroxy-1- CN (phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-33-4 CMF C27 H34 N4 O4 S

Absolute stereochemistry.

CM 2

О== СН- ОН

RN 790252-36-7 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-1-(1-methylethyl)-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-35-6 CMF C31 H42 N4 O5 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН= ОН

RN 790252-38-9 CAPLUS

CN Formic acid, compd. with 1,7-diethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(tetrahydro-ZH-pyran-4-yl)amino]propyl]-1H-pyrrolo[1,2,3ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-37-8 CMF C30 H40 N4 O5 S

CRN 64-18-6 CMF C H2 O2

о== сн-он

790252-40-3 CAPLUS Formic acid, compd. with 3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[(1- $^{\circ}$ CN methylethyl)amino]-1-(phenylmethyl)propyl]-1-methyl-7-(1-methylethyl)-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-39-0 CMF C28 H38 N4 O4 S

Absolute stereochemistry.

CM 2

О— СН— ОН

RN 790252-42-5 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-(cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-3,4-dihydro-1-methyl-7-(1-methylethyl)-1H-pyrrolol1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NNBE)

CM 1

CRN 790252-41-4 CMF C31 H42 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН-ОН

RN 790252-44-7 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-(cyclopropylamino)-2-hydroxy-1-(phenylmethyl)propyl]-3,4-dihydro-1-methyl-7-(1-methylethyl)-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-43-6 CMF C28 H36 N4 O4 S

CRN 64-18-6 CMF C H2 O2

о== сн-он

790252-46-9 CAPLUS Formic acid, compd. with 3,4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethy1)-CN 3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-1-methyl-7-(1-methylethyl)-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-45-8 CMF C30 H40 N4 O5 S

Absolute stereochemistry.

CM

о--- сн-- он

RN 790252-48-1 CAPLUS

CN Formic acid, compd. with 3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-[(phenylmethyl)propyl]-1-methyl-7-(1-methylethyl)-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-47-0 CMF C33 H40 N4 O5 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790252-50-5 CAPLUS

CN Formic acid, compd. with N-{(18,2R)-3-(cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-1,7-diethyl-3,4-dihydro-1H-pyrrolo[1,2,3-ef]-2,1,5benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-49-2 CMF C31 H42 N4 O4 S

CRN 64-18-6 CMF C H2 O2

о == сн - он

CN pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-51-6 CMF C26 H31 F3 N4 O4 S

Absolute stereochemistry.

CM 2

О— СН— ОН

RN 790252-54-9 CAPLUS

CN Formic acid, compd. with 7-ethyl-3, 4-dihydro-N-[(18,2R)-2-hydroxy-3-[(2,2,3,3,3-partafluoropropyl)amino]-1-(phenyl-methyl)propyl]-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NNB)

CM 1

CRN 790252-53-8 CMF C27 H31 F5 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790252-56-1 CAPLUS

CN Formic acid, compd. with N={(18,28)-3-[(cyclopropylmethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-55-0 CMF C28 H36 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн − он

790252-58-3 CAPLUS Formic acid, compd. with N-[(1S,2R)-1-[(3-chlorophenyl)methyl]-3-CN (cyclopropylamino)-2-hydroxypropyl]-7-ethyl-3, 4-dihydro-1-methyl-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-57-2 CMF C27 H33 C1 N4 O4 S

Absolute stereochemistry.

CM

CRN 64-18-6

CMF C H2 O2

O CH OH

RN 790252-60-7 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-1-[(3-chlorophenyl)methyl]-3-(cyclohexylamino)-2-hydroxypropyl]-7-ethyl-3,4-dihydro-1-methyl-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-59-4 CMF C30 H39 C1 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн−он

RN 790252-62-9 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-1-[(3-chlorophenyl)methyl]-2-hydroxy-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-7-ethyl-3, 4-dihydro-1-methyl-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-61-8

CMF C29 H37 C1 N4 O5 S

Absolute stereochemistry.

CM :

CRN 64-18-6 CMF C H2 O2

о== сн-он

RN 790252-64-1 CAPLUS CN Formic acid, compd. with

Formic acid, compd. with N-[(15,2R)-3-(cyclopropylamino)-1-[(3-fluorophenyl)methyl]-2-hydroxypropyl]-7-ethyl-3,4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 790252-63-0

CMF C27 H33 F N4 O4 S Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о= сн-он

RN CN

790252-66-3 CAPLUS Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1- $\mbox{\ }$ (phenylmethyl)-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-1-(2,2,2trifluoroethyl)-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-65-2 CMF C30 H37 F3 N4 O5 S

Absolute stereochemistry.

CM

CRN 64-18-6

CMF C H2 O2

о— сн− он

RN 790252-68-5 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-(cyclohexylamino)-1-[(3-fluorophenyl)methyl]-2-hydroxypropyl]-7-ethyl-3, 4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-67-4 CMF C30 H39 F N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн− он

RN 790252-70-9 CAPLUS

CN Formic acid, compd. with 7-ethyl-N-[(15,2R)-1-[(3-fluorophenyl)methyl]-2hydroxy-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-3,4-dihydro-1-methyl-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-69-6 CMF C29 H37 F N4 O5 S Absolute stereochemistry.

CM :

CRN 64-18-6 CMF C H2 O2

о== сн-он

RN 790252-72-1 CAPLUS
CN Formic acid, compd. with N-[(1S,2R)-3-(cyclohexylamino)-1-[(3,5-

difluorophenyl)methyl]-2-hydroxypropyl]-7-ethyl-3,4-dihydro-1-methyl-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-71-0 CMF C30 H38 F2 N4 O4 S

CRN 64-18-6 CMF C H2 O2

о= сн-он

RN 790252-74-3 CAPLUS

CN Formic acid, compd. with N-[(18,2R)-3-(cyclopropylamino)-1-[(3,5-difluorophenyl)methyl]-2-hydroxypropyl]-7-ethyl-3,4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 790252-73-2

CMF C27 H32 F2 N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о сн−он

RN 790252-75-4 CAPLUS

CN IH-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, N-[(1S,2R)-3-(cyclobutylamino)-2-hydroxy-1-(phenylamethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 790252-77-6 CAPLUS

CN Formic acid, compd. with 7-ethyl-N-[(15,28]-3-[(2-fluoroethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl)-3,4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 790252-76-5 CMF C26 H33 F N4 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

O CH OH

RN 790252-78-7 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, 7-ethyl-3,4-dihydro-N-[(18,2R)-2-hydroxy-1-(phenylmethyl)-3-[(tetrahydro-2,2-dimethyl-2H-pyran-4-yl)amino]propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 790252-79-8 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, N-[(1\$,2R)-3-[(1,1-dimethylethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-,2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 790252-81-2 CAPLUS

CN Formic acid, compd. with 3,4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[([3-(trifluoromethyl)phenyl]methyl]amino]propyl]-1-methyl-7-propyl-1H-pyrrolo[(1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-80-1 CMF C33 H37 F3 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн-он

RN 790252-83-4 CAPLUS

CN Formic acid, compd. with N-{(18,2R)-3-(cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl-1-3,4-dihydro-1-methyl-7-propyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 790252-82-3

CMF C31 H42 N4 O4 S

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10/596,296
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CRN 64-18-6 CMF C H2 O2

O CH OH

RN 790252-85-6 CAPLUS

CN Formic acid, compd. with 3,4-dihydro-N-{(18,2R)-2-hydroxy-1-(phenylmethyl)-3-{(tetrahydro-2-H-pyran-4-yl)amino|propyl-1-methyl-7-propyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-84-5 CMF C30 H40 N4 O5 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн-он

CN

RN 790252-87-8 CAPLUS

Formic acid, compd. with N-[(1S,2R)-3-[[(1-ethyl-1H-pyrazol-4-yl)methyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-3,4-dihydro-1-methyl-7-propyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-86-7 CMF C31 H40 N6 O4 S

CRN 64-18-6 CMF C H2 O2

о == сн - он

790252-89-0 CAPLUS Formic acid, compd. with 1-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1- $\mbox{\ }$ CN (phenylmethyl)-3-[[[3-(trifluoromethyl)phenyl]methyl]amino]propyl]-7propyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-88-9

CMF C34 H39 F3 N4 O4 S

Absolute stereochemistry.

2 CM

CRN 64-18-6

CMF C H2 O2

о = сн - он

RN 790252-91-4 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-(cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-1-ethyl-3,4-dihydro-7-propyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothładiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-90-3 CMF C32 H44 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН= ОН

RN 790252-93-6 CAPLUS

CN Formic acid, compd. with 1-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-7-propyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-92-5 CMF C31 H42 N4 O5 S

CRN 64-18-6 CMF C H2 O2

о= сн-он

790252-96-9 CAPLUS Formic acid, compd. with 1-ethyl-N-[(1S,2R)-3-[[(1-ethyl-1H-pyrazol-4- $^{\prime\prime}]$ CN yl)methyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-3, 4-dihydro-7-propyl-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-95-8 CMF C32 H42 N6 O4 S

Absolute stereochemistry.

CM

CRN 64-18-6 CMF C H2 O2

О— СН— ОН

RN 790252-99-2 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-2hydroxy-3-[(tetrahydro-2H-pyran-4-yl)amino]propyl]-7-ethyl-3, 4-dihydro-1methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790252-98-1 CMF C29 H36 F2 N4 O5 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн= он

RN 790253-02-0 CAPLUS

CN Formic acid, compd. with 7-ethyl-3, 4-dihydro-N-[(15,2R)-2-hydroxy-3-[(2-methoxyethyl)amino]-1-(phenylmethyl)propyl]-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-01-9 CMF C27 H36 N4 O5 S

CM 2

CRN 64-18-6 CMF C H2 O2

о == сн - он

790253-05-3 CAPLUS Formic acid, compd. with 7-ethyl-N-[(1S,2R)-3-(ethylamino)-2-hydroxy-1-(acid, compd.)]CN (phenylmethyl)propyl]-3, 4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-04-2 CMF C26 H34 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2 О== СН- ОН

RN 790253-08-6 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[(1S)1-methylpropyl]amino]-1-(phenylmethyl)propyl]-1-methyl-1H-pyrrolo(1,2,3ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-07-5 CMF C28 H38 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

О== СН= ОН

CN

RN 790253-11-1 CAPLUS

Formic acid, compd. with N-[(15,2R)-3-(butylamino)-2-hydroxy-1-(phenylmethyl)propyl)-7-ethyl-3,4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazeoine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-10-0 CMF C28 H38 N4 O4 S

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790253-13-3 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, 7-ethyl-3,4-dihydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-(2-propyn-1-ylamino)propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 790253-15-5 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, N-[(15,28)-3-(cyclopentylamino)-2-hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

- RN 790253-17-7 CAPLUS
- CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[(2-methylpropyl)amino]-1-(phenylmethyl)propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

- RN 790253-19-9 CAPLUS
- CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, 7-ethyl-3,4-dihydron-I([1,3/R)-2-hydroxy-1-(phenylmethyl)-3-(propylamino)propyl]-1-methyl-,2,2-dioxide (CA INDEX NAME)

- RN 790253-21-3 CAPLUS
- CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[(1R)-1-methylpropyl]amino]-1-

(phenylmethyl)propyl]-1-methyl-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 790253-23-5 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, N-[(15,2R)-3-[(2,2-difluoroethyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 790253-26-8 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(phenylmethyl)amino]propyl]-1-methyl-1H-pyrrolo[1,2,3ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-25-7

CMF C31 H36 N4 O4 S

CRN 64-18-6 CMF C H2 O2

о == сн - он

790253-29-1 CAPLUS Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(2-pyridinylmethyl)amino]propyl]-1-methyl-1H-CN pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-28-0 CMF C30 H35 N5 O4 S

Absolute stereochemistry.

2 CM

CRN 64-18-6 CMF C H2 O2

о = сн - он

RN 790253-32-6 CAPLUS

CN Formic acid, compd. with 7-ethyl-3, 4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(4-pyridinylmethyl)-]maino]propy]1-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NNB)

CM 1

CRN 790253-31-5 CMF C30 H35 N5 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790253-35-9 CAPLUS

CN Formic acid, compd. with 7-ethyl-3, 4-dihydro-M-(118,2R)-2-hydroxy-3-[(2-phenylethyl) amino]-1-(phenylmethyl) propyl]-1-methyl-1H-pyrrolo[1,2,3-et]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-34-8 CMF C32 H38 N4 O4 S

CRN 64-18-6 CMF C H2 O2

о== сн-он

790253-37-1 CAPLUS Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1- $\mbox{\ }$ CN (phenylmethyl)-3-[[[3-(trifluoromethoxy)phenyl]methyl]amino[propyl]-1methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-36-0

CMF C32 H35 F3 N4 O5 S

Absolute stereochemistry.

CM 2

CRN 64-18-6

CMF C H2 O2

О— СН— ОН

RN 790253-39-3 CAPLUS

CN Formic acid, compd. with 7-ethyl-3, 4-dihydro-N-[(1S,2R)-2-hydroxy-1-(phenylmethyl)-3-[(3-pyridinylmethyl)-]maino]propy]1-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NNBE)

CM 1

CRN 790253-38-2 CMF C30 H35 N5 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

o== cн- он

RN 790253-41-7 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[(2-methylphenyl)]methyl]propyl]-1-methyl_Thyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-40-6 CMF C32 H38 N4 O4 S

CRN 64-18-6 CMF C H2 O2

о == сн - он

CN methylphenyl)methyl]amino]-1-(phenylmethyl)propyl]-1-methyl-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 790253-42-8 CMF C32 H38 N4 O4 S

Absolute stereochemistry.

2 CM

CRN 64-18-6 CMF C H2 O2

О— СН— ОН

RN 790253-45-1 CAPLUS

CN Formic acid, compd. with 7-ethyl-3, 4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[(4-methyl-phenyl)-methyl]amino]-1-(phenyl-methyl)-proyl-1-methyl-IH-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-44-0 CMF C32 H38 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790253-47-3 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-[[(1S)-2,3-dihydro-1H-inden-1-y]]amino]-2-hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-46-2 CMF C33 H38 N4 O4 S

CRN 64-18-6 CMF C H2 O2

о == сн - он

790253-49-5 CAPLUS Formic acid, compd. with 1,1-dimethylethyl CN 7-ethyl-3, 4-dihydro-9-[[[(1S, 2R)-2-hydroxy-1-(phenylmethyl)-3-[[[3-(trifluoromethyl)phenyl]methyl]amino]propyl]amino]carbonyl]-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-1-acetate 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-48-4 CMF C37 H43 F3 N4 O6 S

Absolute stereochemistry.

CM

CRN 64-18-6

CMF C H2 O2

о== сн− он

RN 790253-51-9 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(15,2R)-2-hydroxy-1-(phenylmethyl)-3-[[[1-(2,2,2-trifluoroethyl)-1H-pyrazol-4yl]methyl]amino]propyl]-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-50-8 CMF C30 H35 F3 N6 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790253-85-9 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazpine-9-carboxamide, N-[(1S,2R)-3-amino-2-hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

RN 790253-87-1 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-(methylamino)-1-(phenylmethyl)propyl]-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM :

CRN 790253-86-0 CMF C25 H32 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790253-89-3 CAPLUS

CN Formic acid, compd. with 3,4-dihydro-N-[(18,2R)-2-hydroxy-3-(methylamino)-1-(phenylmethyl)propyl)-1-methyl-7-(1-methylethyl)-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 790253-88-2

CMF C26 H34 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790253-91-7 CAPLUS

CN Formic acid, compd. with N=[(1S,2R)-1-[(3-chlorophenyl)methyl]-2-hydroxy-3-(methylamino)propyl]-7-ethyl-3,4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide [1:1] (CA INDEX NAME)

CM :

CRN 790253-90-6 CMF C25 H31 C1 N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

O== CH- OH

RN 790253-93-9 CAPLUS

CN Formic acid, compd. with 7-ethyl-N-[(18,2R)-1-[(3-fluorophenyl)methyl]-2-hydroxy-3-(methylamino)propyl]-3,4-dihydro-1-methyl-lH-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM

CRN 790253-92-8 CMF C25 H31 F N4 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн= он

RN 790253-95-1 CAPLUS

RN 790253-97-3 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-[[(6-bromo-2-pyridinyl)methyl]amino]2-hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1)
(CA INDEX NAME)

CM I

CRN 790253-96-2 CMF C30 H34 Br N5 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790253-99-5 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[[5-[(methylamino)carbonyl]-3-pyridinyl]methyl]amino]-1-(phenylmethyl)propyl]-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790253-98-4 CMF C32 H38 N6 O5 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790254-01-2 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-[([2,2'-bipyridin]-6-ylmethyl)amino]2-hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1)
(CA INDEX NAME)

CM

CRN 790254-00-1 CMF C35 H38 N6 O4 S

CM 2

CRN 64-18-6 CMF C H2 O2

о= сн-он

RN 790254-03-4 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[(6-methyl-2-quinoxalinyl)methyl]amino]-1-(phenylmethyl)propyl]-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790254-02-3 CMF C34 H38 N6 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6

CMF C H2 O2

O CH OH

RN 790254-05-6 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-1 (phenylmethyl)-3-[(3-quinolinylmethyl)aminolpropyl]-1-methyl-1H pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1)
 (CA INDEX NAME)

CM 1

CRN 790254-04-5 CMF C34 H37 N5 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

O== CH= OH

RN 790254-07-8 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[(6-methyl-2-pyridinyl)methyl]amino]-1-(phenylmethyl)propyl]-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790254-06-7 CMF C31 H37 N5 O4 S

CRN 64-18-6 CMF C H2 O2

о == сн - он

790254-09-0 CAPLUS Formic acid, compd. with 7-ethyl-N-[(1S,2R)-3-[[(5-ethyl-2-invariant extension of the compd.]] CN thienyl)methyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-3,4-dihydro-1-methyl-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790254-08-9 CMF C31 H38 N4 O4 S2

Absolute stereochemistry.

CM

CRN 64-18-6 CMF C H2 O2

о--- сн-- он

RN 790254-11-4 CAPLUS

CN Formic acid, compd. with 7-ethyl-3,4-dihydro-N-[(1S,2R)-2-hydroxy-3-[[(5-methyl-2-pyrazinyl)methyl]lamino]-1-(phenylmethyl)propyl]-1-methyl-1H-pyrrolol1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NNB)

CM :

CRN 790254-10-3 CMF C30 H36 N6 O4 S

Absolute stereochemistry.

CM 2

CRN 64-18-6 CMF C H2 O2

о== сн- он

RN 790254-12-5 CAPLUS

CN IH-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, 7-ethyl-N-[(1S,2R)-3-[(3-ethyl-5-isoxazolyl)methyl]amino]-2-hydroxy-1-(phenylmethyl)propyl]-3,4-dihydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

RN 790254-13-6 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, N-[(18,2R)-3-[[(18)-2-(cyclohexylamino)-1-methyl-2-oxoethyl]amino]-2hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

Absolute stereochemistry.

RN 790254-15-8 CAPLUS

CN Formic acid, compd. with N-[(1S,2R)-3-[(4,4-difluorocyclohexyl)amino]-2hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3, 4-dihydro-1-methyl-1Hpyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide 2,2-dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 790254-14-7 CMF C30 H38 F2 N4 O4 S

CRN 64-18-6 CMF C H2 O2

о== сн= он

IT 790255-60-6 790255-61-7 790255-62-8
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of hydroxydiaminopropyl tricyclic indolecarboxamides for treatment of β -amyloid related disease)

RN 790255-60-6 CAPLUS

CN Carbamic acid, [(2R,3S)-3-[[(7-ethyl-3,4-dihydro-1-methyl-2,2-dioxido-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepin-9-yl)carbonyl]amino]-2-hydroxy-4-phenylbutyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 790255-61-7 CAPLUS

CN Carbamic acid, [(2R,3S)-3-[[(7-ethyl-3,4-dihydro-1-methyl-2,2-dioxido-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepin-9-yl)carbonyl]amino]-2-hydroxy-4-phenylbutyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 790255-62-8 CAPLUS

CN Carbamic acid, [(2R,35)-3-[[[3,4-dihydro-1-methyl-7-(1-methylethyl)-2,2-dioxido-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepin-9-yl]carbonyl]amino]-2-hydroxy-4-phenylbutyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Pr-i

```
OH Me

H
N
S
R
N
OP
Ph

1T 790254-27-2P 790254-28-3P 790254-29-4P
790254-30-7P 790254-39-6P 790254-40-9P
790254-42-1P 790254-43-2P 790254-44-3P
790254-45-4P 790254-45-P 790254-46-P
```

790254-48-7P 790254-49-8P 790254-53-4P 790254-63-6P, 790254-55-6P 790254-65-6P 790254-63-6P, 7-Ethyl-3, 4-dihydro-1H-[1,2,5]thiadiazepino[3,4,5-hi]indole-9-carboxylic acid 2,2-dioxide 790254-64-7P,

7-Ethyl-1-methyl-3,4-dihydro-1H-[1,2,5]thiadiazepino[3,4,5-hi]indole-9-carboxylic acid 2,2-dioxide 790254-65-8P,

7-Ethyl-1-phenyl-3,4-dihydro-1H-[1,2,5]thiadiazepino[3,4,5-hi]indole-9-carboxylic acid 2,2-dioxide 790254-67-0P.

 $\label{eq:theory} \begin{array}{lll} 7-\texttt{Ethyl-1}, 3-\texttt{dimethyl-3}, 4-\texttt{dihydro-1H-[1,2,5]} \\ \texttt{thiadiazepino[3,4,5-hi]indole-9-carboxylic acid 2,2-dioxide 790254-68-1P,} \end{array}$

7-Ethyl-1-(phenylmethyl)-3,4-dihydro-1H-[1,2,5]thiadiazepino[3,4,5-hilindole-9-carboxylic acid 2,2-dinyide 790254-70-5P.

hi]indole-9-carboxylic acid 2,2-dioxide 790254-70-5P, 7-Ethyl-1-(1-methylethyl)-3,4-dihydro-1H-[1,2,5]thiadiazepino[3,4,5-

hi]indole-9-carboxylic acid 2,2-dioxide 790254-71-6P, 1,7-Diethyl-3,4-dihydro-1H-[1,2,5]thiadiazepino[3,4,5-hi]indole-9-

carboxylic acid 2,2-dioxide 790254-73-8P,

1-Methyl-7-(1-methylethyl)-3,4-dihydro-1H-[1,2,5]thiadiazepino[3,4,5-hi]indole-9-carboxylic acid 2,2-dioxide 790254-74-9P,

7-Ethyl-1-(2,2,2-trifluoroethyl)-3,4-dihydro-1H-[1,2,5]thiadiazepino[3,4,5-

hi]indole-9-carboxylic acid 2,2-dioxide 790254-75-0P, 1-Methyl-7-propyl-3,4-dihydro-1H-[1,2,5]thiadiazepino[3,4,5-hi]indole-9-

carboxylic acid 2,2-dioxide 790254-78-3P,

1-Ethyl-7-propyl-3,4-dihydro-1H-[1,2,5]thiadiazepino[3,4,5-hi]indole-9-carboxylic acid 2,2-dioxide 790254-79-4P,

 $1-[2-[(1,1-\mathsf{Dimethylethyl})\,\mathsf{oxy}]-2-\mathsf{oxoethyl}]-7-\mathsf{ethyl}-3,4-\mathsf{dihydro}-1\mathsf{H}-1$

[1,2,5]thiadiazepino[3,4,5-hi]indole-9-carboxylic acid 2,2-dioxide RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of hydroxydiaminopropyl tricyclic indolecarboxamides for treatment of $\beta\text{-amyloid}$ related disease)

RN 790254-27-2 CAPLUS CN 1H-Pyrrolo[1,2,3-ef

1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 3,4-dihydro-7-propyl-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-28-3 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 3,4-dihydro-7-(1-methylethyl)-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-29-4 CAPLUS

CN Carbamic acid, [(2R,3S)-4-(3-chlorophenyl)-3-[[(7-ethyl-3,4-dihydro-1-methyl-2,2-dioxido-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepin-9-yl)carbonyl]amino]-2-hydroxybutyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

- RN 790254-30-7 CAPLUS
- CN Carbamic acid, [(2R,3S)-3-[[(7-ethyl-3,4-dihydro-1-methyl-2,2-dioxido-1H-pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepin-9-yl)carbonyl]amino]-4-(3-fluorophenyl)-2-hydroxybutyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

- RN 790254-39-6 CAPLUS
- CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-40-9 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-methyl-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-42-1 CAPLUS CN 1H-Pvrrolo[1,2,3-ef

1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-phenyl-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-43-2 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 3,4-dihydro-1-methyl-7-(1-methylethyl)-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-44-3 CAPLUS
CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid,
3,4-dihydro-1-methyl-7-propyl-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-45-4 CAPLUS CN 1H-Pvrrolo[1,2,3-ef]

N 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-(1-methylethyl)-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-46-5 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 1,7-diethyl-3,4-dihydro-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-47-6 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-(2,2,2-trifluoroethyl)-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-48-7 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 1-ethyl-3,4-dihydro-7-propyl-, methyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-49-8 CAPLUS

RN 790254-53-4 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-, ethyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-55-6 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-methyl-, ethyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-56-7 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-phenyl-, ethyl ester, 2,2-dioxide (CA INDEX NAME)

RN 790254-63-6 CAPLUS CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-,2,2-dioxide (CA INDEX NAME)

RN 790254-64-7 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-methyl-, 2,2-dioxide (CA INDEX NAME)

RN 790254-65-8 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-phenyl-, 2,2-dioxide (CA INDEX NAME)

RN 790254-67-0 CAPLUS
CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid,
7-ethyl-3,4-dihydro-1,3-dimethyl-, 2,2-dioxide (CA INDEX NAME)

RN 790254-68-1 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-(phenylmethyl)-, 2,2-dioxide (CA INDEX NAME)

RN 790254-70-5 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-(1-methylethyl)-, 2,2-dioxide (CA INDEX NAME)

RN 790254-71-6 CAPLUS
CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid,
1,7-diethyl-3,4-dihydro-, 2,2-dioxide (CA INDEX NAME)

RN 790254-73-8 CAPLUS CN 1H-Pvrrolo[1,2,3-ef

IH-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 3,4-dihydro-1-methyl-7-(1-methylethyl)-, 2,2-dioxide (CA INDEX NAME)

RN 790254-74-9 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 7-ethyl-3,4-dihydro-1-(2,2,2-trifluoroethyl)-, 2,2-dioxide (CA INDEX NAME)

RN 790254-75-0 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 3,4-dihydro-1-methyl-7-propyl-, 2,2-dioxide (CA INDEX NAME)

RN 790254-78-3 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxylic acid, 1-ethyl-3,4-dihydro-7-propyl-, 2,2-dioxide (CA INDEX NAME)

RN 790254-79-4 CAPLUS

CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-1-acetic acid, 9-carboxy-7-ethyl-3,4-dihydro-, 1-(1,1-dimethylethyl) ester, 2,2-dioxide (CA INDEX NAME)

3

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:679911 CAPLUS

DOCUMENT NUMBER: 141:374641

TITLE: Behavioural effects of thieno and

pyrazolo[2,1]benzothiazepine derivatives in mice

AUTHOR(S): Exposito-Orta, Maria A.; Albertos, Luz M.; Darias, Victoriano; Sanchez-Mateo, Candelaria C.

CORPORATE SOURCE: Departamento de Farmacologia, Facultad de Farmacia,

Universidad de La Laguna, La Laguna, Tenerife, Spain

SOURCE: Arzneimittel Forschung (2004), 54(7), 365-370

CODEN: ARZNAD; ISSN: 0004-4172

PUBLISHER: Editio Cantor Verlag

DOCUMENT TYPE: Journal LANGUAGE: English

AB Behavioral studies were conducted in mice with a number of hetero[2,1] benotothiazepine derives, analogs of tianeptine. Previously published studies in mice have shown that some of these compds. were effective in the tetrabenazine and Porsolt tests. In the present study, four of the 15 compds. under study potentiated the actions of 5-hydroxytryptophan (5-HTP, 50 mg/kg i,p.), but no significant antagonism of the apomorphine (16 mg/kg s.c.)-induced hypothermia and potentiation of the amphetamine actions was found. Moreover, some of them inhibited the stereotyped behavior and/or climbing behavior of low doses of apomorphine and compound 2 was effective in the plue-maze test. These compds. also produced a slight inhibition of exploratory behavior in the holeboard test. On the other hand, no significant muscle relaxant and anticonvulsant activities were observed at any dose employed. Together, these data suggest that some of the compds. under study combine the antidepressant effects with addnl. neuroleptic or anxiolytic activities in

mice. IT 150555-76-3 150555-77-4 253177-70-7 253177-71-8 253177-72-9 253177-76-3 253177-77-4 253177-78-5 253177-79-6

286854-11-3
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USBS (Uses)

(behavioral effects of thieno and pyrazolo[2,1]benzothiazepine derivs. in mice)

RN 150555-76-3 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepine,

4,9-dihydro-2,9-dimethyl-4-[2-(1-pyrrolidinyl)ethoxy]-, 10,10-dioxide (CA INDEX NAME)

150555-77-4 CAPLUS

Ethanamine, 2-[(5,10-dihydro-5-methyl-4,4-dioxidothieno[3,4-CN c][2,1]benzothiazepin-10-yl)oxy]-N-methyl- (CA INDEX NAME)

253177-70-7 CAPLUS

RN Ethanamine, 2-[(5,10-dihydro-5-methyl-4,4-dioxidothieno[3,4-CN c][2,1]benzothiazepin-10-yl)oxy]-N,N-dimethyl- (CA INDEX NAME)

RN 253177-71-8 CAPLUS

Thieno[3,4-c][2,1]benzothiazepine,

5,10-dihydro-5-methyl-10-[2-(1-pyrrolidinyl)ethoxy]-, 4,4-dioxide (CA INDEX NAME)

253177-72-9 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepine, 5,10-dihydro-5-methyl-10-[2-(1-piperazinyl)ethoxy]-, 4,4-dioxide (CA INDEX NAME)

RN

 $\begin{array}{lll} 253177-76-3 & \texttt{CAPLUS} \\ \texttt{Ethanamine, 2-[(4,9-dihydro-2,9-dimethyl-10,10-dioxido-2H-pyrazolo[3,4-dioxido-2H-pyrazolo])} \end{array}$ CN c][2,1]benzothiazepin-4-yl)oxy]-N-methyl- (CA INDEX NAME)

RN 253177-77-4 CAPLUS

CN Ethanamine, 2-[(4,9-dihydro-2,9-dimethyl-10,10-dioxido-2H-pyrazolo[3,4-c][2,1]benzothiazepin-4-yl)oxy]-N,N-dimethyl- (CA INDEX NAME)

RN 253177-78-5 CAPLUS

CN

O-CH2-CH2-NMe2

2H-Pyrazolo[3,4-c][2,1]benzothiazepine, 4,9-dihydro-2,9-dimethyl-4-[2-(1-piperidinyl)ethoxy]-, 10,10-dioxide (CA INDEX NAME)

RN 253177-79-6 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepine,
 4,9-dihydro-2,9-dimethyl-4-[2-(1-piperazinyl)ethoxy]-, 10,10-dioxide (CA
INDEX NAME)

RN 286854-11-3 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepine, 5,10-dinydro-5-methyl-10-[2-(1-piperidinyl)ethoxy]-, 4,4-dioxide (CA INDEX NAME)

REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L9 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:126817 CAPLUS

DOCUMENT NUMBER: 139:332861

TITLE: Neuropharmacological study of

hetero[2,1]benzothiazepine derivatives analogues of

tianeptine

AUTHOR(S): Sanchez-Mateo, Candelaria C.; Darias, Victoriano; Exposito-Orta, M. Auxiliadora; Albertos, Luz M.

CORPORATE SOURCE: Facultad de Farmacia, Departamento de Farmacologia, Universidad de La Laguna, Tenerife, 38071, Spain

SOURCE: Farmaco (2003), 58(1), 1-10

CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

Neuropharmacol. studies were conducted in mice with a number of hetero[2,1]benzothiazepine derivs., analogs of tianeptine. Seven of the 12 compds. under study potentiated the actions of 5-hydroxytryptophan (5-HTP, 50 mg/kg i.p.) and/or antagonized the hypothermia induced by high doses of apomorphine. Moreover, some of them inhibited the head twitches induced by 5-HTP (250 mg/kg i.p.) and the stereotyped behavior and/or climbing behavior of low doses of apomorphine. These compds. also produced a slight inhibition of exploratory behavior in the holeboard test. On the other hand, no significant muscle relaxant, anticonvulsant and anxiolytic activities were observed at any dose employed. Together, these data suggest that some of the compds. under study exert antidepressant and neuroleptic effects in mice with no muscle relaxant,

anxiolytic and anticonvulsant activities. IT 150555-79-6 616228-16-1 616228-17-2

150555-79-6 616228-16-1 616228-17-2 616228-18-3 616228-19-4 616228-23-0

616228-24-1 616228-25-2 616228-26-3

616228-27-4 616228-28-5 616228-29-6 616228-34-3 616228-35-4 616228-36-5

616228-37-6

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(neuropharmacol. study of hetero[2,1]benzothiazepine derivs. analogs of tianeptine)

RN 150555-79-6 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, 0-[2-(dimethylamino)ethyl]oxime, 10,10-dioxide, (4Z)- (CA INDEX NAME)

CN

RN 616228-16-1 CAPLUS

$$\label{eq:thm:condition} \begin{split} & \text{Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-,} \\ & \text{O-[2-(dimethylamino)ethyl]oxime 4,4-dioxide, (10Z)- (CA INDEX NAME)} \end{split}$$

Double bond geometry as shown.

RN 616228-17-2 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, 0-[2-(1-pyrrolidinyl)ethyl]oxime 4,4-dioxide, (10Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 616228-18-3 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, O-[2-(1-piperidinyl)ethyl]oxime 4,4-dioxide, (10Z)- (CA INDEX NAME)

CN

RN 616228-19-4 CAPLUS

Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, O-[2-(4-morpholinyl)ethyl]oxime 4,4-dioxide, (10Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 616228-23-0 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, O-[2-(1-pyrrolidinyl)ethyl]oxime 10,10-dioxide, (4Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 616228-24-1 CAPLUS

RN 616228-25-2 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, O-[2-(4-morpholinyl)ethyl]oxime 10,10-dioxide, (4Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 616228-26-3 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, O-[2-(dimethylamino)ethyl]oxime 4,4-dioxide, (10E)- (CA INDEX NAME)

Double bond geometry as shown.

RN 616228-27-4 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, O-[2-(1-pyrrolidinyl)ethyl]oxime 4,4-dioxide, (10E)- (CA INDEX NAME)

CN

RN 616228-28-5 CAPLUS

Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, O-[2-(1-piperidinyl)ethyl]oxime 4,4-dioxide, (10E)- (CA INDEX NAME)

Double bond geometry as shown.

RN 616228-29-6 CAPLUS

Double bond geometry as shown.

RN 616228-34-3 CAPLUS

CN

RN 616228-35-4 CAPLUS

2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, O-[2-(1-pyrrolidinyl)ethyl]oxime 10,10-dioxide, (4E)- (CA INDEX NAME)

Double bond geometry as shown.

RN 616228-36-5 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, O-[2-(1-piperidinyl)ethyl]oxime 10,10-dioxide, (4E)- (CA INDEX NAME)

Double bond geometry as shown.

RN 616228-37-6 CAPLUS

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT AR

L9 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:116497 CAPLUS

DOCUMENT NUMBER: 139:159790

TITLE: Psychopharmacological effects of tianeptine analogous

hetero[2,1]benzothiazepine derivatives

AUTHOR(S): Sanchez-Mateo, Candelaria C.; Darias, Victoriano;

Albertos, Luz M.; Exposito-Orta, Maria A.

CORPORATE SOURCE: Departamento de Farmacologia, Facultad de Farmacia, Universidad de La Laguna, La Laguna, Spain

SOURCE: Arzneimittel-Forschung (2003), 53(1), 12-20

CODEN: ARZNAD; ISSN: 0004-4172

PUBLISHER: Editio Cantor Verlag
DOCUMENT TYPE: Journal

DOCUMENT TYPE: Journal LANGUAGE: English

The psychopharmacol. effects of a number of thieno and pyrazolo[2,1]benzothiazepine derivs. as well as several synthetic intermediate compds. were investigated in mice. Previously published studies in mice have shown that some of these compds. were effective in the tetrabenazine and Porsolt tests. In the present study, 7 of the 15 compds, under study clearly antagonized the apomorphine (16 mg/kg s.c.)-induced hypothermia, but no significant potentiation of the 5-hydroxytryptophan (5-HTP) and amphetamine actions was found. Five of them inhibited the syndrome induced by 5-HTP (250 mg/kg i.p.). Moreover, some of them were effective in the plus-maze test and antagonized the apomorphine (3 mg/kg s.c.)-induced effects. These compds. produced a moderate inhibition of exploratory behavior in the holeboard test, but they had no significant muscle relaxant and anticonvulsant activities. The results indicate that some of the compds. under study combine a spectrum of antidepressant, anxiolytic and neuroleptic properties in mice with a lack of muscle relaxant and anticonvulsant activities.

IT 153757-46-1 155144-46-0 155144-49-3 198212-74-7 198212-80-5 198212-84-9

204853-98-5 204853-99-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(psychopharmacol. effects of tianeptine hetero[2,1]benzothiazepine derivs.)

RN 153757-46-1 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, 4,4-dioxide (CA INDEX NAME)

RN 155144-46-0 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 9-methyl-, 10,10-dioxide (CA INDEX NAME)

RN 155144-49-3 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, 10,10-dioxide (CA INDEX NAME)

RN 198212-74-7 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, oxime, 4,4-dioxide (CA INDEX NAME)

RN 198212-80-5 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10-ol, 5,10-dihydro-5-methyl-, 4,4-dioxide (CA INDEX NAME)

RN 198212-84-9 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4-ol, 4,9-dihydro-2,9-dimethyl-, 10,10-dioxide (CA INDEX NAME)

RN 204853-98-5 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, oxime, 10,10-dioxide (CA INDEX NAME)

RN 204853-99-6 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 9-methyl-, oxime, 10,10-dioxide (CA INDEX NAME)

REFERENCE COUNT:

25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L9 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:369035 CAPLUS

DOCUMENT NUMBER: 133:135298

TITLE: Synthesis of new thieno- and

pyrazolo[2,1]benzothiazepine derivatives with
potential antidepressant properties

AUTHOR(S): Vega, S.; Diaz, J. A.; Darias, V.; Mateo, C. C.

Sanchez
CORPORATE SOURCE: Instituto de Ouimica Medica, CSIC, Madrid, 28006,

Spain

SOURCE: Journal of Heterocyclic Chemistry (2000), 37(2), 389-393

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

DOCUMENT TYPE: Journal LANGUAGE: English

AB In this paper we describe a series of new thieno- and

pyrazolo[2,1]benzothiazepine derivs., which were synthesized by two different methods, both starting from tricyclic alcs. Several components of this series were effective p. o. (per os, orally) in different pharmacol, tests currently employed in the evaluation of antidepressant

activity. IT 150832-64-7P 253177-78-5P 253177-79-6P 286854-09-9P 286854-10-2P 286854-12-4P 286854-13-5P 286854-20-4P

286854-21-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); FREP (Preparation)

(preparation and antidepressant properties of thieno- and pyrazolobenzothiazepines)

RN 150832-63-6 CAPLUS

INDEX NAME)

1

Ethanamine, 2-[(5,10-dihydro-5-methyl-4,4-dioxidothieno[3,4-c][2,1]benzothiazepin-10-yl)oxy]-N-methyl-, (2Z)-2-butenedioate (1:1) (CA)

CM

CN

CRN 150555-77-4 CMF C15 H18 N2 O3 S2

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

HO₂C CO2H

RN 150832-64-7 CAPLUS

CN Butanedioic acid, compd. with 4,9-dihydro-2,9-dimethyl-4-[2-(1pyrrolidinyl)ethoxyl-2H-pyrazolo[3,4-c][2,1]benzothiazepine dioxide (1:1) (CA INDEX NAME)

CM 1

CRN 150555-76-3 CMF C18 H24 N4 O3 S

CM 2

CRN 110-15-6

CMF C4 H6 O4

HO2C-CH2-CH2-CO2H

253177-78-5 CAPLUS

2H-Pyrazolo[3,4-c][2,1]benzothiazepine, 4,9-dihydro-2,9-dimethyl-4-[2-(1-piperidinyl)ethoxy]-, 10,10-dioxide (CA INDEX NAME)

CN

253177-79-6 CAPLUS

CN

2H-Pyrazolo[3,4-c][2,1]benzothiazepine, 4,9-dihydro-2,9-dimethyl-4-[2-(1-piperazinyl)ethoxy]-, 10,10-dioxide (CA INDEX NAME)

RN

286854-09-9 CAPLUS Ethanamine, 2-[(5,10-dihydro-5-methyl-4,4-dioxidothieno[3,4-CN c][2,1]benzothiazepin-10-yl)oxy]-N,N-dimethyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

```
CRN 253177-70-7
CMF C16 H20 N2 O3 S2
```

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

CN

RN 286854-10-2 CAPLUS

Thieno[3,4-c][2,1]benzothiazepine, 5,10-dihydro-5-methyl-10-[2-(1-pyrrolidinyl)ethoxy]-, 4,4-dioxide, (22)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 253177-71-8 CMF C18 H22 N2 O3 S2

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 286854-12-4 CAPLUS CN Thieno[3,4-c][2,1]b

Thieno[3,4-c][2,1]benzothiazepine, 5,10-dihydro-5-methyl-10-[2-(1-piperidinyl)ethoxy]-, 4,4-dioxide, (22)-2-butenedioate (1:1) (901) (CA INDEX NAME)

CM 1

CRN 286854-11-3 CMF C19 H24 N2 O3 S2

CM

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

CN

RN 286854-13-5 CAPLUS

Thieno[3,4-c][2,1]benzothiazepine, 5,10-dihydro-5-methyl-10-[2-(1-piperazinyl)ethoxy]-, 4,4-dioxide, (22)-2-butenedioate (1:2) (901) (CA INDEX NAME)

CM 1

CRN 253177-72-9 CMF C18 H23 N3 O3 S2

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 286854-20-4 CAPLUS
CN Ethanamine, 2-[(4,9-dihydro-2,9-dimethyl-10,10-dioxido-2H-pyrazolo[3,4-c][2,1]benzothiazepin-4-yl)oxy]-N-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 253177-76-3 CMF C15 H20 N4 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 286854-21-5 CAPLUS
CN Ethanamine, 2-[(4,9-dihydro-2,9-dimethyl-10,10-dioxido-2H-pyrazolo[3,4-

c][2,1]benzothiazepin-4-yl)oxy]-N,N-dimethyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 253177-77-4 CMF C16 H22 N4 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

CMF C4 H4 O4

IT 198212-80-5

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation and antidepressant properties of thieno- and pyrazolobenzothiazepines)

RN 198212-80-5 CAPLUS CN Thieno(3.4-c)(2.11b)

Thieno[3,4-c][2,1]benzothiazepin-10-ol, 5,10-dihydro-5-methyl-, 4,4-dioxide (CA INDEX NAME)

IT 150555-84-3P 198212-84-9P 286854-08-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and antidepressant properties of thieno- and pyrazolobenzothiazepines)

RN 150555-84-3 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepine,

10-(2-bromoethoxy)-5,10-dihydro-5-methyl-, 4,4-dioxide (CA INDEX NAME)

RN 198212-84-9 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4-ol, 4,9-dihydro-2,9-dimethyl-, 10,10-dioxide (CA INDEX NAME)

RN 286854-08-8 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepine, 4-(2-bromoethoxy)-4,9-dihydro-2,9-dimethyl-, 10,10-dioxide (CA INDEX NAME)

REFERENCE COUNT:

10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 10 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:705433 CAPLUS

DOCUMENT NUMBER: 132:58715

TITLE: New thieno and pyrazolo[2,1]benzothiazepine

derivatives with antidepressant activity

AUTHOR(S): Darias, V.; Sanchez-Mateo, C. C.; Exposito-Orta, M.

A.; Albertos, L. M.; Diaz, J. A.; Vega, S.

CORPORATE SOURCE: Departamento de Farmacologia, Facultad de Farmacia,

Universidad de La Laguna, Spain SOURCE: Pharmazie (1999), 54(10), 783-784 CODEN: PHARAT; ISSN: 0031-7144

PUBLISHER: Govi-Verlag Pharmazeutischer Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

Several compds. of the hetero[2,1]benzothiazepine series under study were effective orally in different animal models predictive of antidepressant activity, like the Porsolt test and antagonism to tetrabenazine-induced effects. Two thieno derivs., di-Me thieno[3,4-c]benzothiazepine and thieno[3,2-c]benzothiazepine, were in this order the most effective, with activities similar or better than those of reference drugs (imipramine and tianeptine). The pyrazolo[3,4-c] derivs., however, showed a lower degree of activity in these tests.

150555-76-3 150555-77-4 253177-70-7 253177-71-8 253177-72-9 253177-76-3

253177-77-4 253177-78-5 253177-79-6 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(thieno and pyrazolo[2,1]benzothiazepine derivs. with antidepressant activity)

150555-76-3 CAPLUS RN

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepine,

4,9-dihydro-2,9-dimethyl-4-[2-(1-pyrrolidinyl)ethoxy]-, 10,10-dioxide (CA INDEX NAME)

- RN 150555-77-4 CAPLUS
- Ethanamine, 2-[(5,10-dihydro-5-methyl-4,4-dioxidothieno[3,4-

c][2,1]benzothiazepin-10-y1)oxy]-N-methy1- (CA INDEX NAME)

RN 253177-70-7 CAPLUS

CN Ethanamine, 2-[(5,10-dihydro-5-methyl-4,4-dioxidothieno[3,4-c][2,1]benzothiazepin-10-yl)oxy]-N,N-dimethyl- (CA INDEX NAME)

0-CH₂-CH₂-NMe₂

RN 253177-71-8 CAPLUS CN Thieno[3,4-c][2,1]benzothi

 $\label{eq:capacity} \begin{tabular}{ll} Thieno[3,4-c][2,1] benzothiazepine, \\ 5,10-dihydro-5-methyl-10-[2-(1-pyrrolidinyl)ethoxy]-, 4,4-dioxide (CA INDEX NAME) \\ \end{tabular}$

- RN 253177-72-9 CAPLUS
- CN Thieno[3,4-c][2,1]benzothiazepine, 5,10-dihydro-5-methyl-10-[2-(1-piperazinyl)ethoxy]-, 4,4-dioxide (CA INDEX NAME)

- RN 253177-76-3 CAPLUS
- CN Ethanamine, 2-[(4,9-dihydro-2,9-dimethyl-10,10-dioxido-2H-pyrazolo[3,4-c][2,1]benzothiazepin-4-yl)oxy]-N-methyl- (CA INDEX NAME)

- RN 253177-77-4 CAPLUS
- CN Ethanamine, 2-[(4,9-dihydro-2,9-dimethyl-10,10-dioxido-2H-pyrazolo[3,4-c][2,1]benzothiazepin-4-yl)oxy]-N,N-dimethyl- (CA INDEX NAME)

RN 253177-78-5 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepine, 4,9-dihydro-2,9-dimethyl-4-[2-(1-piperidinyl)ethoxy]-, 10,10-dioxide (CA INDEX NAME)

RN 253177-79-6 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepine, 4,9-dihydro-2,9-dimethyl-4-[2-(1-piperazinyl)ethoxy]-, 10,10-dioxide (CA INDEX NAME)

REFERENCE COUNT: 13

.3 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/596.296

ANSWER 11 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:116568 CAPLUS DOCUMENT NUMBER: 128:238994

ORIGINAL REFERENCE NO.: 128:47137a,47140a

TITLE: Antidepressant activity of new hetero[2,1]benzothiazepine derivatives

AUTHOR(S): Vega, S.; Diaz, J. A.; Darias, V.; Sanchez Mateo, C.

C.; Albertos, L. M.

CORPORATE SOURCE: Instituto Ouimica Medica, Madrid, E-28006, Spain

SOURCE: Pharmazie (1998), 53(2), 130-134

CODEN: PHARAT; ISSN: 0031-7144 PUBLISHER: Govi-Verlag Pharmazeutischer Verlag English

DOCUMENT TYPE: Journal

LANGUAGE:

A number of thieno and pyrazolo[2,1]benzothiazepine derivs. as well as several synthetic intermediate compds. were tested for acute toxicity and antidepressant activity in mice. Some of these compds. were effective in the tetrabenazine and Porsolt tests.

153757-46-1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses) (antidepressant activity of new hetero[2,1]benzothiazepine derivs.)

153757-46-1 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, 4,4-dioxide (CA INDEX NAME)

155144-46-0P 155144-49-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (antidepressant activity of new hetero[2,1]benzothiazepine derivs.)

RN 155144-46-0 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 9-methyl-, 10,10-dioxide (CA INDEX NAME)

RN 155144-49-3 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, 10,10-dioxide (CA INDEX NAME)

IT 198212-74-7P 198212-80-5P 198212-84-9P 204853-98-5P 204853-99-6P

RI. BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BJOL (Biological study); PREP (Preparation); USES (Uses)

(antidepressant activity of new hetero[2,1]benzothiazepine derivs.) RN 198212-74-7 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, oxime, 4,4-dioxide (CA INDEX NAME)

RN 198212-80-5 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10-ol, 5,10-dihydro-5-methyl-, 4,4-dioxide (CA INDEX NAME)

RN 198212-84-9 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4-o1, 4,9-dihydro-2,9-dimethyl-, 10,10-dioxide (CA INDEX NAME)

RN 204853-98-5 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, oxime, 10,10-dioxide (CA INDEX NAME)

RN 204853-99-6 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 9-methyl-, oxime, 10,10-dioxide (CA INDEX NAME)

10/596.296

1.9 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:644488 CAPLUS DOCUMENT NUMBER: 127:346367

ORIGINAL REFERENCE NO.: 127:67963a,67966a

Synthesis of new hetero[2,1]benzothiazepine TITLE:

derivatives

AUTHOR(S): Vega, Salvador; Diaz, Juan A.

CORPORATE SOURCE: Instituto de Ouimica Medica, CSIC, Madrid, 28006,

SOURCE: Journal of Heterocyclic Chemistry (1997), 34(4),

1191-1194

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation DOCUMENT TYPE: Journal

LANGUAGE: English

Ι

AΒ As part of an investigation directed to the search of new neurotropic agents, a number of hydroxy and hydroximino derivs. of the novel thieno and pyrazolo[2,1]benzothiazepine ring systems, e.g., I, were prepared Assignments of the Z and E hydroximino isomers were performed by study of their 1H and 13C NMR spectra and NOE expts.

153757-46-1 155144-46-0 155144-49-3

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of heterobenzothiazepine derivs.)

RN 153757-46-1 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, 4,4-dioxide (CA INDEX NAME)

155144-46-0 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 9-methyl-, 10,10-dioxide (CA INDEX NAME)

RN 155144-49-3 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, 10,10-dioxide (CA INDEX NAME)

IT 150555-86-5P 198212-74-7P 198212-76-9P 198212-77-0P 198212-78-1P 198212-80-5P

198212-84-9P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of heterobenzothiazepine derivs.)
RN 150555-86-5 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, oxime, 10,10-dioxide, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 198212-74-7 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, oxime, 4,4-dioxide (CA INDEX NAME)

RN 198212-76-9 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, oxime, 10,10-dioxide, (4E)- (CA INDEX NAME)

Double bond geometry as shown.

RN 198212-77-0 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 9-methyl-, oxime, 10,10-dioxide, (4E)- (CA INDEX NAME)

Double bond geometry as shown.

RN 198212-78-1 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 9-methyl-, oxime, 10,10-dioxide, (4Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 198212-80-5 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10-ol, 5,10-dihydro-5-methyl-, 4,4-dioxide (CA INDEX NAME)

RN 198212-84-9 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4-ol, 4,9-dihydro-2,9-dimethyl-, 10,10-dioxide (CA INDEX NAME)

REFERENCE COUNT:

15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/596.296

ANSWER 13 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:495431 CAPLUS DOCUMENT NUMBER: 125 - 184907

ORIGINAL REFERENCE NO.: 125:34303a,34306a

Synthesis and antidepressant evaluation of new TITLE:

hetero[2,1]benzothiazepine derivatives

AUTHOR(S): Diaz, Juan A.; Vega, Salvador; Exposito, Maria A.; Sanchez Mateo, Candelaria C.; Darias, Victoriano

CORPORATE SOURCE: Inst. Quimica Medica, CSIC, Madrid, 28006, Spain

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1996),

329(7), 352-360

CODEN: ARPMAS; ISSN: 0365-6233

PUBLISHER: DOCUMENT TYPE: Journal

LANGUAGE . English

As a part of a research program directed to the discovery of novel antidepressant agents, a series of new hetero[2,1]benzothiazepine derivs. was synthesized. Some of these compds. antagonized the ptosis and motor depression induced by tetrabenazine and were also active in the Porsolt forced swimming test. These activities, however, were lower than those elicited by the reference drugs viloxazine and tianeptine. Structure activity relations are discussed.

181145-37-9P 181145-38-0P 181145-39-1P 181145-40-4P 181145-46-0P 181145-48-2P

181145-50-6P 181145-52-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(synthesis and antidepressant evaluation of new

hetero[2,1]benzothiazepine derivs.)

181145-37-9 CAPLUS RN

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-,

O-[2-(dimethylamino)ethyl]oxime, 4,4-dioxide, hydrochloride (1:1) (CA INDEX NAME)

N-0-CH2-CH2-NMe2

HC1

181145-38-0 CAPLUS CN

Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, O-[2-(1-pyrrolidinyl)ethyl]oxime, 4,4-dioxide, hydrochloride (1:1) (CA INDEX NAME)

RN 181145-39-1 CAPLUS

RN 181145-40-4 CAPLUS

Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, O-[2-(4-morpholinyl)ethyl]oxime, 4,4-dioxide, hydrochloride (1:1) (CA INDEX NAME)

181145-46-0 CAPLUS CN

2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, O-[2-(dimethylamino)ethyl]oxime, 10,10-dioxide, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

Me

CRN 181145-45-9 CMF C16 H21 N5 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-,

O-[2-(1-piperidinyl)ethyl]oxime, 10,10-dioxide, (22)-2-butenedioate (1:1)

Page 437

181145-50-6 CAPLUS

RN

CN

(9CI) (CA INDEX NAME) CM 1 CRN 181145-49-3 CMF C19 H25 N5 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 181145-52-8 CAPLUS CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, O-[2-(4-morpholinyl)ethyl]oxime, 10,10-dioxide, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME) CM 1

CRN 181145-51-7 CMF C18 H23 N5 O4 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

10/596.296

T.9 ANSWER 14 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:187571 CAPLUS

DOCUMENT NUMBER: 124:317117

ORIGINAL REFERENCE NO.: 124:58813a

Preparation and regiochemical assignments of new TITLE:

pyrazolo[3, 4-c][2,1]benzothiazepines

AUTHOR(S): Arranz, Ester; Diaz, Juan A.; Morante, Esther; Perez,

Carmen; Vega, Salvador

CORPORATE SOURCE: Instituto de Ouimica Medica, CSIC, Madrid, 28006,

Spain

SOURCE: Journal of Heterocyclic Chemistry (1996), 33(1), 151-6

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation Journal

DOCUMENT TYPE: LANGUAGE: English

GI

- AB The preparation of new pyrazolo[3,4-c][2,1]benzothiazepines I (R = Me, Et, CH2Ph, etc.) and II (R = Me, Et, CH2Ph) substituted at the nitrogen atoms of the pyrazole moiety is described. It was carried out by reaction of the 4,9-dihydro-9-methyl-4,10,10-trioxo-1(2)H-pyrazolo[3,4c][2,1]benzothiazepine with several alkylating agents under both classical and phase-transfer catalysis (PTC) conditions. Assignments of the N-alkyl regioisomers obtained were performed by study of their 1H NMR spectra and
 - NOE expts. 155144-46-0
 - RL: RCT (Reactant); RACT (Reactant or reagent)
 - (preparation and regiochem. of pyrazolobenzothiazepines)
- RN 155144-46-0 CAPLUS
- CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 9-methyl-, 10,10-dioxide (CA INDEX NAME)

IT 155144-49-3P 176383-35-0P 176383-36-1P
176383-37-2P 176383-38-3P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and regiochem. of pyrazolobenzothiazepines)

- RN 155144-49-3 CAPLUS
- CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, 10,10-dioxide (CA INDEX NAME)

- RN 176383-35-0 CAPLUS
- CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2-ethyl-9-methyl-, 10,10-dioxide (CA INDEX NAME)

- RN 176383-36-1 CAPLUS
- CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 9-methyl-2-(phenylmethyl)-, 10,10-dioxide (CA INDEX NAME)

- RN 176383-37-2 CAPLUS
- CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one,

9-methyl-2-(2-phenylethyl)-, 10,10-dioxide (CA INDEX NAME)

RN 176383-38-3 CAPLUS

CN 2H-Fyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2-cyclohexyl-9-methyl-, 10,10-dioxide (CA INDEX NAME)

ANSWER 15 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN 1.9 ACCESSION NUMBER: 1994:409363 CAPLUS

DOCUMENT NUMBER: 121:9363

ORIGINAL REFERENCE NO.: 121:1981a,1984a

TITLE: Synthesis of 1H- and

2H-pyrazolo[3,4-c][2,1]benzothiazepines

AUTHOR(S): Diaz, Juan A.; Vega, Salvador

CORPORATE SOURCE: Inst. Quim. Med., CSIC, Madrid, 28006, Spain

SOURCE: Journal of Heterocyclic Chemistry (1994), 31(1), 93-6

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Starting from Et chlorosulfonylpyrazole-4-carboxylates the authors have carried out the synthesis of ketones I and II which are the first two structures of the novel 1H- and 2H-pyrazolo[3,4-c][2,1]benzothiazepine ring systems.

ΙT 155144-49-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 155144-49-3 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, 10,10-dioxide (CA INDEX NAME)

10/596.296

ANSWER 16 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN 1994:323617 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER: 120:323617

ORIGINAL REFERENCE NO.: 120:56945a,56948a

TITLE: Process for preparation of

trioxopyrazolo[2,1]benzothiazepines as potential

therapeutics

INVENTOR(S): Vega Noverola, Salvador; Diaz Martin, Juan Antonio

PATENT ASSIGNEE(S): Consejo Superior de Investigaciones Cientificas, Spain

SOURCE: Span., 5 pp. CODEN: SPXXAD DOCUMENT TYPE: Patent

LANGUAGE: Spanish

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	ΕN		NO			
ES	20	46	94	1		

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 2046941	A1	19940201	ES 1991-2366	19911024
ES 2046941	B1	19940816		
PRIORITY APPLN. INFO.:			ES 1991-2366	19911024
OTHER SOURCE(S):	CASRE	ACT 120:32361	17; MARPAT 120:323617	

- Title compds. and analogs I [R1 = H, (un)substituted alkyl or arylalkyl; R2 = H, halo, NO2, amino, sulfonamido, CF3; X = N, NMe, NH, CH; Y = N, NMe, NH, CH, CMe; Z = N, CH, CMe] are prepared by a claimed 3-step process, illustrated below. I are useful as intermediates, or potentially as antibacterial agents, diuretics, or antihypertensives. Sulfonamidation of Et 3(5)-(chlorosulfonyl)pyrazole-4-carboxylate with PhNHMe in refluxing THF gave sulfonamide II (R = Et), which was hydrolyzed by refluxing 1N KOH to give the corresponding acid II (R = H). Cyclization of the acid by polyphosphoric acid in boiling xylene gave I (R1 = Me, R2 = H, X = N, Y = NH, Z = CH).
- 155144-46-0P 155144-49-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate or potential therapeutic)

- RN 155144-46-0 CAPLUS
- 2H-Pvrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 9-methvl-, 10,10-dioxide (CA INDEX NAME)

RN 155144-49-3 CAPLUS

CN 2H-Pyrazolo(3,4-c)(2,1)benzothiazepin-4(9H)-one, 2,9-dimethyl-, 10,10-dioxide (CA INDEX NAME)

L9 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1994:217612 CAPLUS

DOCUMENT NUMBER: 120:217612

ORIGINAL REFERENCE NO.: 120:38645a,38648a

TITLE:

Synthesis of thieno[3,4-c] and thieno[3,2-c][2,1]benzothiazepines

AUTHOR(S): Vega, Salvador; Diaz, Juan A.

CORPORATE SOURCE: Inst. Ouim. Med., CSIC, Madrid, 28006, Spain

SOURCE: Journal of Heterocyclic Chemistry (1993), 30(6),

1509-12 CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English GT

Ι

AB Starting from [4,3-c] and [3,2-c] Me (chlorosulfonyl)thiophenecarboxylates the synthesis of ketones I (X = S, Y = CH; X = CH, Y = S) is described. These compds. are the first two representatives of the new thieno[3,4-c] and thieno[3,2-c]benzothiazepine ring systems. The formation of Me

3-chlorosulfonvlthiophene-2-carboxvlate is also revised. ΙT 153757-46-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 153757-46-1 CAPLUS

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, 4,4-dioxide (CA INDEX NAME)

ANSWER 18 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:649978 CAPLUS DOCUMENT NUMBER: 119:249978

ORIGINAL REFERENCE NO.: 119:44605a,44608a

Preparation of pharmacologically active tricyclic TITLE: benzotriazepine derivatives

INVENTOR(S): Vega Noverola, Salvador; Diaz Martin, Juan Antonio

PATENT ASSIGNEE(S): (Csie and Adir et Cie), Spain; Adir et Cie

SOURCE: Eur. Pat. Appl., 25 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patient.

LANGUAGE: English FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 547705	A1	19930623	EP 1992-203913	19921215
R: AT, BE, CH,	DE, DK,	ES, FR, GB	, GR, IE, IT, LI, LU,	, MC, NL, PT, SE
ES 2040629	A1	19931016	ES 1991-2818	19911218
ES 2040629	B1	19940616		
CA 2085705	A1	19930619	CA 1992-2085705	19921217
ZA 9209777	A	19930623	ZA 1992-9777	19921217
AU 9230303	A	19930624	AU 1992-30303	19921218
JP 06001794	A	19940111	JP 1992-338491	19921218
PRIORITY APPLN. INFO.:			ES 1991-2818	A 19911218
OTHER SOURCE(S):	MARPAT	119:249978		
CT				

Title compds. I [X = N, S, HN, alkyl-N, alkylaryl-N, HC; Y = N, S, HN, alkyl-N, alkylaryl-N, HC; Z = N, S, HC, alkyl-C, aryl-C; R1 = H, alkyl (substituted) arylalkyl; R2 = lH, halo, O2N, (substituted) amine, NC, SO2NH, F3C, C1-36 alkv1, C1-36 alkoxy; R3, R4 = H, halo, HO, alkoxy, HS, (substituted) amino, Het-(C1-5 alkv1)-T wherein T = 0, N, S, n = 0, 1, Het = (substituted) heterocyclyl], are prepared NaBH4 was added to 5,10-dihydro-5-methyl-4,4,10-trioxothieno[3,2-c][2,1]-benzothiazopine in MeOH to give I (X = Y = HC, Z = S, R1 = Me, R2 = R4 = H, R3 = HO) which at 100 mg/kg, p.o., showed inhibition of pain in the Siegmund test.

150555-76-3P 150555-77-4P 150555-79-6P 150555-81-0P 150555-88-7P 150832-63-6P

150832-64-7P 150832-65-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as drug)

150555-76-3 CAPLUS RN

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepine, 4,9-dihydro-2,9-dimethyl-4-[2-(1-pyrrolidinyl)ethoxy]-, 10,10-dioxide (CA INBEX NAME)

RN 150555-77-4 CAPLUS

CN Ethanamine, 2-[(5,10-dihydro-5-methyl-4,4-dioxidothieno[3,4-c][2,1]benzothiazepin-10-yl)oxy]-N-methyl- (CA INDEX NAME)

RN 150555-79-6 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, O-[2-(dimethylamino)ethyl]oxime, 10,10-dioxide, (4Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 150555-81-0 CAPLUS

CN 1-Propanamine, N,N-dimethyl-3-(5-methyl-4,4-dioxidothieno[3,4-c][2,1]benzothiazepin-10(5H)-ylidene)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 150555-88-7 CAPLUS

CN 1-Propanamine, N,N-dimethyl-3-(5-methyl-4,4-dioxidothieno[3,4-c][2,1]benzothiazepin-10(5H)-ylidene)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 150832-63-6 CAPLUS

CN Ethanamine, 2-[(5,10-dihydro-5-methyl-4,4-dioxidothieno[3,4-c)[2,1]benzothiazepin-10-yl)oxy]-N-methyl-, (22)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 150555-77-4 CMF C15 H18 N2 O3 S2

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

CN

RN 150832-64-7 CAPLUS

Butanedioic acid, compd. with 4,9-dihydro-2,9-dimethyl-4-[2-(1pyrrolidiny1)ethoxy]-2H-pyrazolo[3,4-c][2,1]benzothiazepine dioxide (1:1) (CA INDEX NAME)

CM

CRN 150555-76-3 CMF C18 H24 N4 O3 S

CM

CRN 110-15-6 CMF C4 H6 O4

HO2C-CH2-CH2-CO2H

RN 150832-65-8 CAPLUS

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, 0-(2-(dimethylamino)ethyl]oxime, 10,10-dioxide, (4Z)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM

CRN 150555-79-6 CMF C16 H21 N5 O3 S

Double bond geometry as shown.

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

ΙT 150555-84-3 150555-86-5

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, in preparation of drugs)

150555-84-3 CAPLUS RN

CN Thieno[3, 4-c][2,1]benzothiazepine,

10-(2-bromoethoxy)-5,10-dihydro-5-methyl-, 4,4-dioxide (CA INDEX NAME)

RN

150555-86-5 CAPLUS CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, oxime, 10,10-dioxide, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L9 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:214543 CAPLUS

DOCUMENT NUMBER: 116:214543

ORIGINAL REFERENCE NO.: 116:36365a,36368a

TITLE: Preparation of new trioxothienobenzothiazepines
INVENTOR(S): Vega Noverola, Salvador; Diaz Martin, Juan Antonio

PATENT ASSIGNEE(S): Consejo Superior de Investigaciones Cientificas, Spain SOURCE: Span., 4 pp.

CODEN: SPXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Spanish

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 2021548	A6	19911101	ES 1990-1576	19900607
PRIORITY APPLN. INFO.:			ES 1990-1576	19900607
OTHER SOURCE(S):	MARPAT	116:214543		

GI

AB Title heterocycles I [Rl = H, alkyl, (un)substituted aralkyl; R2 = H, halo, NO2, amino, sulfonamido, CF3; X = S, CH, CMe, CPh; Y = S, CH, CMe] are prepared in 3 steps: (1) reaction of corresponding sulfonyl chlorides and anilines in the presence of a base to give sulfonamides II (R = undefined esterifying group); (2) alkaline hydrolysis of the esters to give acids II (R = H); and (3) intramol. cyclization of the acids in the presence of a dehydrating agent. I are useful as psychotropics, antibacterials, diuretics, antihypertensives, etc. (no data). For example, PhNHMe and 3-(chlorosulfonyl)-2-(methoxycarbonyl)thiophene reacted in THF to give II (R = RI = Me, R2 = H, X = CH, Y = S), which was hydrolyzed to II (R = H, others as above) in refluxing IN KOH. Cyclization by polyphosphoric acid in refluxing PhMe gave I (RI = Me, R2 = H, X = CH, Y = S). The isomeric I (RI = Me, R2 = H, X = S, Y = CH) was prepared identically.

II

IT 140947-43-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

- (preparation of, as potential drug) RN 140947-43-9 CAPLUS
- CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl- (CA INDEX NAME)

ANSWER 144 OF 144 REGISTRY COPYRIGHT 2008 ACS on STN L7

RN 181145-45-9 REGISTRY

ED Entered STN: 24 Sep 1996

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, O-[2-(dimethylamino)ethyl]oxime, 10,10-dioxide (CA INDEX NAME)

MF C16 H21 N5 O3 S

CI COM CA

SR

N-0-CH2-CH2-NMe2

- L7 ANSWER 139 OF 144 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 751459-97-9 REGISTRY
- ED Entered STN: 26 Sep 2004
- CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, O-[2-(1-piperidinyl)ethyl]oxime 4,4-dioxide (CA INDEX NAME) OTHER CA INDEX NAMES:
- CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, 0-[2-(1-piperidinyl)ethyl]oxime, 4,4-dioxide (9CI)
- MF C19 H23 N3 O3 S2
- CI COM
- SR CA

- L7 ANSWER 140 OF 144 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 733721-49-8 REGISTRY
- ED Entered STN: 27 Aug 2004
- CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, 0-[2-(1-pyrrolidinyl)ethyl]oxime 4,4-dioxide (CA INDEX NAME) OTHER CA INDEX NAMES:
- CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, O-[2-(1-pyrrolidinyl)ethyl]oxime, 4,4-dioxide (9CI)
- MF C18 H21 N3 O3 S2
- CI COM
- SR CA

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L7 ANSWER 141 OF 144 REGISTRY COPYRIGHT 2008 ACS on STN
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RN 181145-51-7 REGISTRY

ED Entered STN: 24 Sep 1996

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, O-[2-(4-morpholinyl)ethyl]oxime, 10,10-dioxide (CA INDEX NAME)

MF C18 H23 N5 04 S

CI COM SR CA

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L7 ANSWER 142 OF 144 REGISTRY COPYRIGHT 2008 ACS on STN
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RN 181145-49-3 REGISTRY

ED Entered STN: 24 Sep 1996

CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, O-[2-(1-piperidinyl)ethyl]oxime, 10,10-dioxide (CA INDEX NAME)

MF C19 H25 N5 O3 S

CI COM SR CA

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L7
    ANSWER 143 OF 144 REGISTRY COPYRIGHT 2008 ACS on STN
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RN 181145-47-1 REGISTRY

ED Entered STN: 24 Sep 1996

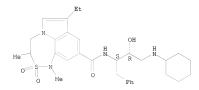
CN 2H-Pyrazolo[3,4-c][2,1]benzothiazepin-4(9H)-one, 2,9-dimethyl-, O-[2-(1-pyrrolidinyl)ethyl]oxime, 10,10-dioxide (CA INDEX NAME)

MF C18 H23 N5 O3 S

CI COM SR CA

- L7 ANSWER 135 OF 144 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 790252-11-8 REGISTRY
- ED Entered STN: 29 Nov 2004
- CN 1H-Pyrrolo[1,2,3-ef]-2,1,5-benzothiadiazepine-9-carboxamide, N-[(15,2R)-3-(cyclohexylamino)-2-hydroxy-1-(phenylmethyl)propyl]-7-ethyl-3,4-dihydro-1,3-dimethyl-,2,2-dioxide (CA INDEX NAME)
- FS STEREOSEARCH
- MF C31 H42 N4 O4 S
- CI COM
- SR CA

Absolute stereochemistry.



- L7 ANSWER 136 OF 144 REGISTRY COPYRIGHT 2008 ACS on STN
- RN 790252-07-2 REGISTRY
- ED Entered STN: 29 Nov 2004
- FS STEREOSEARCH
- MF C33 H37 F3 N4 O4 S
- CI COM SR CA

Absolute stereochemistry.

L7 ANSWER 137 OF 144 REGISTRY COPYRIGHT 2008 ACS on STN

RN 784118-55-4 REGISTRY

ED Entered STN: 19 Nov 2004

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, 0-[2-(4-morpholinyl)ethyl]oxime 4,4-dioxide (CA INDEX NAME) OTHER CA INDEX NAMES:

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-,
O-[2-(4-morpholinyl)ethyl]oxime, 4,4-dioxide (9CI)

MF C18 H21 N3 O4 S2

CI COM

SR CA

L7 ANSWER 138 OF 144 REGISTRY COPYRIGHT 2008 ACS on STN

RN 760924-40-1 REGISTRY

ED Entered STN: 11 Oct 2004

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-, O-[2-(dimethylamino)ethyl]oxime 4,4-dioxide (CA INDEX NAME) OTHER CA INDEX NAMES:

CN Thieno[3,4-c][2,1]benzothiazepin-10(5H)-one, 5-methyl-,
O-[2-(dimethylamino)ethyl]oxime, 4,4-dioxide (9CI)

MF C16 H19 N3 O3 S2

CI COM

SR CA